```
(FILE 'HOME' ENTERED AT 13:54:39 ON 31 MAY 2011)
     FILE 'REGISTRY' ENTERED AT 13:54:48 ON 31 MAY 2011
                E (104-45-0)/RN
                E = (135-02-4)/RN
                E (151-10-0)/RN
                E DIHYDROANETHOLE/CN
L1
              1 S E35
                E O-ANISALDEHYDE/CN
L2
              1 S E47
                E 1,3-DIMETHOXYBENZENE/CN
L3
              1 S E59
                E 2-HYDROXYACETOPHENONE/CN
L4
              1 S E71
                E 2-METHOXYACETOPHENONE/CN
L5
              1 S E83
     FILE 'HOME' ENTERED AT 14:00:21 ON 31 MAY 2011
     FILE 'STNGUIDE' ENTERED AT 14:13:17 ON 31 MAY 2011
     FILE 'FOMAD, FROSTI, FSTA' ENTERED AT 14:19:56 ON 31 MAY 2011
              0 S L1
L6
              0 S L2
L7
              0 S L3
L8
L9
              0 S L4
L10
              0 S L5
L11
            146 S METHYL SALICYLATE
L12
             42 S P-ANISALDEHYDE
L13
              3 S O-ANISALDEHYDE
     FILE 'MEDLINE, HCAPLUS' ENTERED AT 14:24:22 ON 31 MAY 2011
           1505 S O-METHOXYBENZALDEHYDE OR O-ANISALDEHYDE
L14
L15
              3 S L14 (L) APPLE JUICE
L16
              3 S L2 (L) APPLE JUICE
L17
              0 S L15 NOT L16
L18
             19 S L1 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
            15 S L2 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L20
             29 S L3 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L21
             6 S L4 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L22
             1 S L5 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L23
             1 S L22 AND PY<2004
             4 S L21 AND PY<2004
L24
             12 S L20 AND PY<2004
L25
             6 S L19 AND PY<2004
L26
L27
             10 S L18 AND PY<2004
             31 S L23 OR L24 OR L25 OR L26 OR L27
L28
=> s 128 and (flavor? or flavour?)
           20 L28 AND (FLAVOR? OR FLAVOUR?)
L29
=> d ibib iabs kwic hit 1-20
THE ESTIMATED COST FOR THIS REQUEST IS 72.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) / N: y
L29 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER:
                         2003:791065 HCAPLUS
DOCUMENT NUMBER:
                         140:41025
TITLE:
                         Truffle aroma characterization by headspace
```

solid-phase microextraction

AUTHOR(S): Diaz, P.; Ibanez, E.; Senorans, F. J.; Reglero, G. CORPORATE SOURCE: Universidad Catolica de Avila, Avila, 05005, Spain SOURCE: Journal of Chromatography, A (2003), 1017(1-2),

207-214

CODEN: JCRAEY; ISSN: 0021-9673

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

ABSTRACT:

In the present study, a headspace solid-phase microextn. (HS-SPME) combined to gas chromatog.-mass spectrometry (GC-MS) was used to fully characterize aroma of truffles of different species. A fiber of medium polarity (for flavors) was used to avoid discrimination towards very non-polar and polar volatile compds. In a previous work, extraction conditions were optimized by means of an exptl. design leading to the following conditions that were used in the present study: extraction temperature, 53 °C; extraction time, 13.6 min; and equilibrium time, 5 min.

A comparison among different truffles species has been established in terms of qual. and quant. differences on volatile composition By using the optimal extraction

conditions and GC-MS it was possible to identify 89 compds. in 2 different truffle species such as Tuber aestivum and Tuber melanosporum. An attempt was made to be able to determine the influence of different geog. origins on the aroma fraction of such fungi.

- SO Journal of Chromatography, A (2003), 1017(1-2), 207-214 CODEN: JCRAEY; ISSN: 0021-9673
- AB . . . chromatog.-mass spectrometry (GC-MS) was used to fully characterize aroma of truffles of different species. A fiber of medium polarity (for flavors) was used to avoid discrimination towards very non-polar and polar volatile compds. In a previous work, extraction conditions were optimized. . .
- IT Flavor
 Odor and Odorous substances
 Tuber aestivum
 Tuber melanosporum
 Tuberaceae
 Volatile substances

(truffle aroma characterization by headspace solid-phase microextn.) 60-12-8, Phenylethanol 64-19-7, Acetic acid, biological studies 66-25-1, Hexanal 67-64-1, 2-Propanone, biological studies Sulfinylbismethane, biological studies 75-07-0, Acetaldehyde, biological 75-18-3, Dimethyl sulfide 78-83-1, 2-Methyl-1-propanol, studies biological studies 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological 79-10-7, 2-Propenoic acid, biological studies 88-69-7, studies 91-16-7, 1,2-Dimethoxybenzene 2-(1-Methylethyl)phenol Naphthalene, biological studies 93-15-2, 1,2-Dimethoxy-4-(2-propenyl)benzene 95-47-6, 1,2-Dimethylbenzene, biological studies 95-63-6, 1,2,4-Trimethylbenzene 96-17-3, 2-Methylbutanal 96-48-0, 2(3H)-Dihydrofuranone 98-01-1, 2-Furancarboxaldehyde, biological studies 100-41-4, Ethylbenzene, biological studies 100-52-7, Benzaldehyde, biological studies 100-66-3, Methoxybenzene, biological studies 100-84-5, $1-\texttt{Methoxy-3-methylbenzene} \qquad 104-46-1 \text{, } 1-\texttt{Methoxy-4-(1-propenyl)benzene}$ 106-42-3, 1,4-Dimethylbenzene, biological 104-76-7, 2-Ethyl-1-hexanol studies 106-44-5, p-Cresol, biological studies 106-68-3, 3-Octanone 108-38-3, 1,3-Dimethylbenzene, biological studies 108-64-5, Ethyl 3-methylbutanoate 108-88-3, Methylbenzene, biological studies 108-95-2, Phenol, biological studies 111-13-7, 2-Octanone 111-27-3, 1-Hexanol, biological studies 111-70-6, 1-Heptanol 111-71-7, Heptanal

```
112-12-9, 2-Undecanone
                             112-31-2, Decanal 112-54-9, Dodecanal
    122-78-1, Phenylacetaldehyde 123-38-6, Propanal, biological studies
                                 124-13-0, Octanal 124-19-6, Nonanal
    123-51-3, 3-Methyl-1-butanol
    128-37-0, 2,6-Bis(1,1-dimethylethyl)-4-methylphenol, biological studies
    137-32-6, 2-Methyl-1-butanol 141-78-6, Ethyl acetate, biological studies
    151-10-0, 1,3-Dimethoxybenzene 494-99-5, 3,4-Dimethoxytoluene
    513-86-0, 3-Hydroxy-2-butanone 565-62-8, 3-Methyl-3-penten-2-one
                               589-59-3, 2-Methylpropyl-3-methylbutanoate
    585-25-1, 2,3-Octanedione
    589-98-0, 3-Octanol 590-86-3, 3-Methylbutanal 620-83-7,
    1-Methyl-4-(phenylmethyl)benzene 624-92-0, Dimethyl disulfide
    625-33-2, 3-Penten-2-one 1115-11-3, 2-Methyl-2-butenal 1453-58-3
    1481-93-2, 4-Hydroxychroman 1669-44-9, 3-Octen-2-one 1758-88-9,
    2-Ethyl-1,4-dimethylbenzene 2050-01-3, 3-Methylbutyl-2-methylpropanoate
    2363-88-4, 2,4-Decadienal 2363-89-5, 2-Octenal 2445-67-2 2445-78-5,
    2-Methylbutyl-2-methylbutanoate 2463-63-0, 2-Heptenal 3391-86-4,
    1-Octen-3-ol 3658-80-8, Dimethyl trisulfide 3777-69-3, 2-Pentylfuran
    4170-30-3, 2-Butenal 4411-89-6 4536-23-6, 2-Methylhexanoic acid
               6750-03-4, 2,4-Nonadienal 6836-38-0, 6-Dodecanol
    5920-29-6
    14044-41-8
                15706-73-7, Butyl 2-methylbutanoate 18217-12-4,
    5-Methyl-2-heptanone 19872-52-7, 4-Mercapto-4-methyl-2-pentanone
    24599-58-4, 2,5-Dimethoxytoluene 25415-62-7, Pentyl 3-methylbutanoate
    34314-83-5, 2,3-Dihydro-4-methylfuran 83861-74-9, Octa-1,5-dien-3-ol
    120550-70-1
    RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical
    study); BIOL (Biological study)
        (truffle aroma characterization by headspace solid-phase
       microextn.)
OS.CITING REF COUNT:
                        34
                              THERE ARE 34 CAPLUS RECORDS THAT CITE THIS
                              RECORD (34 CITINGS)
REFERENCE COUNT:
                        22
                              THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
    Journal of Chromatography, A (2003), 1017(1-2), 207-214
    CODEN: JCRAEY; ISSN: 0021-9673
    In the present study, a headspace solid-phase microextn. (HS-SPME)
    combined to gas chromatog.-mass spectrometry (GC-MS) was used to fully
    characterize aroma of truffles of different species. A fiber of medium
    polarity (for flavors) was used to avoid discrimination towards very
    non-polar and polar volatile compds. In a previous work, extraction conditions
    were optimized by means of an exptl. design leading to the following
    conditions that were used in the present study: extraction temperature, 53 °C;
    extraction time, 13.6 min; and equilibrium time, 5 min. A comparison among
    different truffles species has been established in terms of qual. and
    quant. differences on volatile composition By using the optimal extraction
    conditions and GC-MS it was possible to identify 89 compds. in 2 different
    truffle species such as Tuber aestivum and Tuber melanosporum. An attempt
    was made to be able to determine the influence of different geog. origins on
    the aroma fraction of such fungi.
    Flavor
    Odor and Odorous substances
    Tuber aestivum
    Tuber melanosporum
    Tuberaceae
    Volatile substances
        (truffle aroma characterization by headspace solid-phase microextn.)
    60-12-8, Phenylethanol 64-19-7, Acetic acid, biological studies
    66-25-1, Hexanal 67-64-1, 2-Propanone, biological studies
                                                                 67 - 68 - 5,
    Sulfinylbismethane, biological studies 75-07-0, Acetaldehyde, biological
             75-18-3, Dimethyl sulfide 78-83-1, 2-Methyl-1-propanol,
    studies
    biological studies 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological
             79-10-7, 2-Propenoic acid, biological studies 88-69-7,
    studies
    2-(1-Methylethyl)phenol 91-16-7, 1,2-Dimethoxybenzene
```

SO

AΒ

ΙT

```
Naphthalene, biological studies 93-15-2,
    1,2-Dimethoxy-4-(2-propenyl)benzene 95-47-6, 1,2-Dimethylbenzene,
    biological studies 95-63-6, 1,2,4-Trimethylbenzene 96-17-3,
    2-Methylbutanal 96-48-0, 2(3H)-Dihydrofuranone 98-01-1,
    2-Furancarboxaldehyde, biological studies 100-41-4, Ethylbenzene,
    biological studies 100-52-7, Benzaldehyde, biological studies
    100-66-3, Methoxybenzene, biological studies
                                                  100-84-5,
    1-Methoxy-3-methylbenzene 104-46-1, 1-Methoxy-4-(1-propenyl)benzene
    104-76-7, 2-Ethyl-1-hexanol 106-42-3, 1,4-Dimethylbenzene, biological
    studies 106-44-5, p-Cresol, biological studies 106-68-3, 3-Octanone
    108-38-3, 1,3-Dimethylbenzene, biological studies 108-64-5, Ethyl
    3-methylbutanoate 108-88-3, Methylbenzene, biological studies
    108-95-2, Phenol, biological studies 111-13-7, 2-Octanone 111-27-3,
    1-Hexanol, biological studies 111-70-6, 1-Heptanol 111-71-7, Heptanal
    112-12-9, 2-Undecanone 112-31-2, Decanal 112-54-9, Dodecanal
    122-78-1, Phenylacetaldehyde 123-38-6, Propanal, biological studies
    123-51-3, 3-Methyl-1-butanol
                                 124-13-0, Octanal 124-19-6, Nonanal
    128-37-0, 2,6-Bis(1,1-dimethylethyl)-4-methylphenol, biological studies
    137-32-6, 2-Methyl-1-butanol 141-78-6, Ethyl acetate, biological studies
    151-10-0, 1,3-Dimethoxybenzene 494-99-5, 3,4-Dimethoxytoluene
    513-86-0, 3-Hydroxy-2-butanone 565-62-8, 3-Methyl-3-penten-2-one
    585-25-1, 2,3-Octanedione 589-59-3, 2-Methylpropyl-3-methylbutanoate 589-98-0, 3-Octanol 590-86-3, 3-Methylbutanal 620-83-7,
    1-Methyl-4-(phenylmethyl)benzene 624-92-0, Dimethyl disulfide
    625-33-2, 3-Penten-2-one 1115-11-3, 2-Methyl-2-butenal 1453-58-3
    2363-88-4, 2,4-Decadienal 2363-89-5, 2-Octenal 2445-67-2 2445-78-5,
    2-Methylbutyl-2-methylbutanoate 2463-63-0, 2-Heptenal 3391-86-4,
    1-Octen-3-ol 3658-80-8, Dimethyl trisulfide 3777-69-3, 2-Pentylfuran
                                     4536-23-6, 2-Methylhexanoic acid
    4170-30-3, 2-Butenal 4411-89-6
              6750-03-4, 2,4-Nonadienal
                                           6836-38-0, 6-Dodecanol
    5920-29-6
    14044-41-8
                15706-73-7, Butyl 2-methylbutanoate 18217-12-4,
    5-Methyl-2-heptanone
                         19872-52-7, 4-Mercapto-4-methyl-2-pentanone
    24599-58-4, 2,5-Dimethoxytoluene 25415-62-7, Pentyl 3-methylbutanoate
    34314-83-5, 2,3-Dihydro-4-methylfuran
                                           83861-74-9, Octa-1,5-dien-3-ol
    120550-70-1
    RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical
    study); BIOL (Biological study)
        (truffle aroma characterization by headspace solid-phase
       microextn.)
L29 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER:
                        2003:230629 HCAPLUS
DOCUMENT NUMBER:
                        138:384323
TITLE:
                        Investigation of beer flavor by gas
                        chromatography-olfactometry
                        Murakami, A. A.; Goldstein, H.; Navarro, A.;
AUTHOR(S):
                        Seabrooks, J. R.; Ryder, D. S.
CORPORATE SOURCE:
                        Miller Brewing Company, Milwaukee, WI, 53201, USA
SOURCE:
                        Journal of the American Society of Brewing Chemists
                        (2003), 61(1), 23-32
CODEN: JSBCD3; ISSN: 0361-0470
                        American Society of Brewing Chemists, Inc.
```

ABSTRACT:
Gas chromatog.-olfactometry (GC-O) is an anal. technique for evaluating the aroma characteristics of volatile constituents separated by gas chromatog. (GC). This article presents 3 case studies employing the GC-O technique in brewing, including investigation of kettle hop aroma, an off-aroma in beer, and

Journal English

PUBLISHER: DOCUMENT TYPE:

LANGUAGE:

aged-beer aroma. The kettle hop aroma was studied using a GC-O technique called CharmAnal. (DATU, Inc., Geneva, NY) and beer strongly hopped with Oregon Cascade hop pellets at 45 min before end of kettle boil. CharmAnal. can quantitate the intensity of an aroma detected at a sniff port. It revealed that linalool was an important aroma compound in hopped beer and that phenylethyl alc. and two Co-eluting, tentatively identified constituents were important aroma compds. in hopped and unhopped beers. In a second study, GC-O was employed for investigating an objectionable aroma described as medicinal/phenolic/Band-Aid in a production beer. GC-O was able to reveal the eluting off-odor that matched the off-aroma character in the beer. In a third case study, a quant. GC-O technique called AromaTrax (Microanalytics, Round Rock, TX) was employed to determine aged-beer aroma. This technique revealed that quant. changes of many minor components possessing unpleasant aroma notes, particularly the carboxylic acids, were involved in aged-beer aroma.

```
Investigation of beer flavor by gas chromatography-olfactometry
ΤТ
     Journal of the American Society of Brewing Chemists (2003), 61(1), 23-32
SO
     CODEN: JSBCD3; ISSN: 0361-0470
     beer flavor detection gas chromatog olfactometry
ST
ΙT
     Brewing
     Gas chromatography
     Humulus
     Odor and Odorous substances
     Volatile substances
        (beer flavor by gas chromatog.-olfactometry)
ΙT
     Beer analysis
        (beer flavor by gas chromatog.-olfactometry in)
ΙT
     Odor and Odorous substances
        (off-odor; beer flavor by gas chromatog.-olfactometry)
     60-12-8, Phenylethyl alcohol 71-41-0, Amyl alcohol, biological studies
ΤТ
     78-70-6, Linalool 97-62-1, Ethyl 2-methylpropanoate 98-00-0,
     2-Furanmethanol 103-36-6, Ethyl cinnamate 103-45-7, 2-Phenylethyl
             104-67-6, \gamma-Undecalactone
                                         105-54-4, Ethyl butyrate
     acetate
     106-24-1, trans-Geraniol 106-25-2, Nerol 110-38-3, Ethyl decanoate
     118-71-8, Maltol 121-33-5, Vanillin 123-51-3, 3-Methyl-1-butanol
     123-66-0, Ethyl hexanoate
                                123-92-2, Isoamyl acetate
                                                           503-74-2,
                          527-35-5, 2,3,5,6-Tetramethylphenol
     3-Methylbutyric acid
                                                                  551-93-9,
     o-Aminoacetophenone 934-34-9, 2-(3H)-Benzothiazolone 1450-72-2,
     1-(2-Hydroxy-5-methylphenyl)ethanone
                                           3658-80-8, Dimethyl trisulfide
     4079-52-1, 2-Methoxyacetophenone
                                        6617-49-8
                                                    7786-61-0,
                      23726-93-4, \beta-Damascenone
     4-Vinylquaiacol
     RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical
     study); BIOL (Biological study)
        (beer flavor by gas chromatog.-olfactometry)
OS.CITING REF COUNT:
                               THERE ARE 11 CAPLUS RECORDS THAT CITE THIS
                         11
                               RECORD (11 CITINGS)
REFERENCE COUNT:
                               THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
                         18
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
ΤI
     Investigation of beer flavor by gas chromatography-olfactometry
     Journal of the American Society of Brewing Chemists (2003), 61(1), 23-32
SO
     CODEN: JSBCD3; ISSN: 0361-0470
ST
     beer flavor detection gas chromatog olfactometry
ΙT
     Brewing
     Gas chromatography
     Humulus
     Odor and Odorous substances
     Volatile substances
        (beer flavor by gas chromatog.-olfactometry)
ΤТ
     Beer analysis
        (beer flavor by gas chromatog.-olfactometry in)
     Odor and Odorous substances
ΤТ
```

(off-odor; beer flavor by gas chromatog.-olfactometry) 60-12-8, Phenylethyl alcohol 71-41-0, Amyl alcohol, biological studies ΤТ 78-70-6, Linalool 97-62-1, Ethyl 2-methylpropanoate 98-00-0, 2-Furanmethanol 103-36-6, Ethyl cinnamate 103-45-7, 2-Phenylethyl acetate 104-67-6, γ -Undecalactone 105-54-4, Ethyl butyrate 106-24-1, trans-Geraniol 106-25-2, Nerol 110-38-3, Ethyl decanoate 118-71-8, Maltol 121-33-5, Vanillin 123-51-3, 3-Methyl-1-butanol 123-66-0, Ethyl hexanoate 123-92-2, Isoamyl acetate 503-74-2, 527-35-5, 2,3,5,6-Tetramethylphenol 3-Methylbutyric acid o-Aminoacetophenone 934-34-9, 2-(3H)-Benzothiazolone 1450-72-2, 1-(2-Hydroxy-5-methylphenyl)ethanone 3658-80-8, Dimethyl trisulfide 4079-52-1, 2-Methoxyacetophenone 6617-49-8 7786-61-0, 4-Vinylguaiacol 23726-93-4, β -Damascenone RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study) (beer flavor by gas chromatog.-olfactometry)

L29 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2001:912026 HCAPLUS

DOCUMENT NUMBER: 136:324259

TITLE: Headspace aroma of "wild onion" trees

AUTHOR(S): Yang, Xiaogen; Josephson, Dave; Peppet, Jeff;

Eilerman, Robert; Grab, Willi; Gassenmeier, Klaus Givaudan Flavors Corp., Cincinnati, OH, 45216, USA Special Publication - Royal Society of Chemistry

(2001), 274 (Food Flavors and Chemistry), 266-273

CODEN: SROCDO; ISSN: 0260-6291

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

ABSTRACT:

SOURCE:

CORPORATE SOURCE:

In the Gabonese rain forest, there are at least 4 types of trees whose bark have strong garlic-like or onion-like odor. They are often called "wild onion trees". These trees were identified as Afrostyrax kamerunensis Huac., Scorodophloeus zenkere Huac., Hua gabonii Huac., and Afrostyrax lepidophylleus Huac. The bark of the trees are used for cooking. The leaves and seeds of H. gabonii and A. lepidophylleus, and the roots from young trees of A. kamerunensis are also used in flavoring sauces. In addition, the bark also are used for medicinal purposes. The volatile components of freshly cut bark of 3 species: A. kamerunensis, S. zenkere, H. gabonii were collected and analyzed. Many sulfur-containing compds. were present in the headspace. The character impact compds. were identified as di-Me disulfide, 2,3,5-trithiahexane, 2,4,6-trithiaheptane, and 2,4-dithiapentane by GC sniffing.

- SO Special Publication Royal Society of Chemistry (2001), 274(Food Flavors and Chemistry), 266-273
 CODEN: SROCDO; ISSN: 0260-6291
- AB . . . seeds of H. gabonii and A. lepidophylleus, and the roots from young trees of A. kamerunensis are also used in flavoring sauces. In addition, the bark also are used for medicinal purposes. The volatile components of freshly cut bark of 3. . .
- 60-12-8, Phenylethyl alcohol 64-17-5, Ethanol, biological studies ΙT 64-19-7, Acetic acid, biological studies 65-85-0, Benzoic acid, 66-25-1, n-Hexanal 67-68-5, Dimethyl sulfoxide, 67-71-0, Dimethyl sulfone 68-11-1, Mercaptoacet biological studies biological studies 68-11-1, Mercaptoacetic 71-36-3, Butan-1-ol, biological studies acid, biological studies 71-41-0, Amyl alcohol, biological studies 74-93-1, Methanethiol, biological studies 78-93-3, Methyl ethyl ketone, biological studies 80-56-8, α -Pinene 87-20-7, Iso-Amyl salicylate 87 - 44 - 5 β -Caryophyllene 88-84-6, β -Guaiene 91-57-6, 2-Methylnaphthalene 95-16-9, Benzothiazole 98-01-1, Furfural,

```
biological studies 98-86-2, Acetophenone, biological studies 99-85-4,
\gamma-Terpinene 99-87-6, p-Cymene 100-47-0, Benzonitrile, biological
        100-51-6, Benzyl alcohol, biological studies 100-52-7,
studies
Benzaldehyde, biological studies 100-66-3, Anisole, biological studies
104-76-7, 2-Ethylhexan-1-ol 106-21-8, 3,7-Dimethyl-1-octanol 106-68-3,
3-Octanone 107-89-1, 3-Hydroxybutanal 107-92-6, n-Butyric acid,
biological studies 107-93-7, trans-2-Butenoic acid 108-95-2, Phenol,
biological studies 110-93-0, 6-Methylhept-5-en-2-one 111-27-3,
1-Hexanol, biological studies 111-71-7, Heptanal 112-05-0, Nonanoic
      112-32-3, n-Octyl formate 112-88-9, 1-Octadecene 112-92-5,
Octadecanol 118-56-9, Homomenthyl salicylate 118-60-5, 2-Ethylhexyl
salicylate 119-61-9, Benzophenone, biological studies 122-00-9,
p-Methylacetophenone 122-78-1, Phenyl acetaldehyde 123-35-3, Myrcene
123-42-2, 4-Hydroxy-4-methyl-2-pentanone 123-51-3, Iso-Amyl alcohol
123-72-8, Butanal 124-07-2, Octanoic acid, biological studies
124-13-0, Octanal 124-19-6, Nonanal 126-33-0, Tetrahydrothiophene,
1,1,dioxide 127-91-3, \beta-Pinene 128-37-0, Ionol, biological
studies 137-32-6, 2-Methylbutan-1-ol 138-86-3, Limonene
Caproic acid, biological studies 142-91-6, Isopropyl palmitate
149-57-5, 2-Ethylhexanoic acid 289-16-7, 1,2,4-Trithiolane 291-22-5, 1,2,4,5-Tetrathiane 292-45-5, 1,2,4,6-Tetrathiepane 470-82-6,
1,8-Cineole 473-13-2, \alpha-Selinene 483-76-1, \delta-Cadinene
483-78-3, Cadalene 502-61-4, Farnesene 506-42-3,
trans-9-Octadecen-1-ol 512-61-8, Santalene 513-86-0, Acetoin 514-51-2, \beta-Patchoulene 536-74-3, Phenylacetylene 541-85-5,
5-Methyl-3-heptanone 555-10-2, \beta-Phellandrene 579-07-7,
1-Phenyl-1, 2-propanedione 582-24-1,
\alpha-Hydroxyacetophenone 586-62-9, Terpinolene 589-82-2, 3-Heptanol
589-98-0, Octan-3-ol 616-25-1, Pent-1-en-3-ol 617-94-7,
\alpha, \alpha-Dimethylbenzenemethanol 623-36-9 624-92-0, Dimethyl
disulfide 625-28-5, 3-Methyl butanenitrile 644-30-4, \alpha-Curcumene
732-26-3, Tri-tert-butyl phenol 926-37-4, 4,4-Dimethylpent-2-enal
928-96-1, cis-Hex-3-en-1-ol 930-60-9, 2-Cyclopentene-1,4-dione
933-48-2, Trixanol 1454-85-9, 1-Heptadecanol 1576-95-0, cis-2-Pentenol
1618-26-4, 2,4-Dithiapentane 1620-98-0,
3,5-Di-tert-butyl-4-hydroxybenzaldehyde 1741-83-9, 2-Thiaheptane
1795-15-9, Octylcyclohexane 1879-07-8, cis-p-Menth-8-ene 1879-09-0,
6-tert-Butyl-2, 4-dimethyl phenol 2277-20-5, 6-Nonenal, (E)-
                                                                 2314-48-9,
Carbonotrithioic acid dimethyl ester 2436-90-0, Citronellene
3338-55-4, cis-\beta-Ocimene 3387-41-5, Sabinene 3391-86-4,
1-Octen-3-ol
             3491-57-4 3592-19-6 3658-80-8, Dimethyl trisulfide
3777-69-3, 2-Pentylfuran 3913-02-8, 2-Butyl octanol 4130-42-1,
2,6-Bis(1,1-dimethylethyl)-4-ethylphenol 4170-30-3, 2-Butenal
4312-99-6, 1-Octen-3-one 4630-07-3, Valencene
                                                 4829-04-3,
1,3-Dithiolane
                 5008-72-0 5418-86-0 6540-86-9, 2,4,6-Trithiaheptane
          6728-26-3, trans-Hex-2-en-1-al 6753-98-6, Humulene
6617-49-8
6938-51-8, 2-Octylbenzoate 10522-26-6, 2-Methyl-1-undecanol 13877-93-5
15193-25-6, o-Menth-8-ene 16225-26-6, 3,5-Di-tert-butylbenzoic acid
16630-52-7, 3-Methylthiobutanal 17066-67-0, \beta-Selinene
17283-81-7, Dihydro \beta-ionone 17699-14-8, \alpha-Cubebene
18794-84-8, Trans-\beta-Farnesene
                               19780-25-7, 2-Ethyl-2-butenal
20068-02-4 23986-74-5, Germacrene D 27070-58-2, Octadecene
27251-68-9, Pentadecene 27625-35-0, 3-Methylbutyl 2-methylbutyrate 33577-16-1 38514-13-5, 3-Ethyl-4-methyl-1-pentanol 38634-59-2,
Methylthiomethyl acetyl sulfide 42474-44-2, 2,3,5-Trithiahexane
51154-96-2, Massoialactone 58809-73-7, 2-Methylthiopropionic acid
66537-39-1
             66537-40-4 80466-34-8, 2,4-Hexadienal 85544-38-3,
2,4,5,7-Tetrathiaoctane 103240-92-2 117210-66-9 119117-00-9
415686-96-3
             415687-00-2
RL: ANT (Analyte); BSU (Biological study, unclassified); OCU (Occurrence,
unclassified); ANST (Analytical study); BIOL (Biological study); OCCU
```

(Occurrence)

(headspace aroma of wild onion trees)

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

- SO Special Publication Royal Society of Chemistry (2001), 274(Food Flavors and Chemistry), 266-273
 CODEN: SROCDO; ISSN: 0260-6291
- AB In the Gabonese rain forest, there are at least 4 types of trees whose bark have strong garlic-like or onion-like odor. They are often called "wild onion trees". These trees were identified as Afrostyrax kamerunensis Huac., Scorodophloeus zenkere Huac., Hua gabonii Huac., and Afrostyrax lepidophylleus Huac. The bark of the trees are used for cooking. The leaves and seeds of H. gabonii and A. lepidophylleus, and the roots from young trees of A. kamerunensis are also used in flavoring sauces. In addition, the bark also are used for medicinal purposes. The volatile components of freshly cut bark of 3 species: A. kamerunensis, S. zenkere, H. gabonii were collected and analyzed. Many sulfur-containing compds. were present in the headspace. The character impact compds. were identified as di-Me disulfide, 2,3,5-trithiahexane, 2,4,6-trithiaheptane, and 2,4-dithiapentane by GC sniffing.
- 60-12-8, Phenylethyl alcohol 64-17-5, Ethanol, biological studies ΙT 64-19-7, Acetic acid, biological studies 65-85-0, Benzoic acid, biological studies 66-25-1, n-Hexanal 67-68-5, Dimethyl sulfoxide, biological studies 67-71-0, Dimethyl sulfone 68-11-1, Mercaptoacetic acid, biological studies 71-36-3, Butan-1-ol, biological studies 71-41-0, Amyl alcohol, biological studies 74-93-1, Methanethiol, biological studies 78-93-3, Methyl ethyl ketone, biological studies 80-56-8, α -Pinene 87-20-7, Iso-Amyl salicylate 87-44-5, β -Caryophyllene 88-84-6, β -Guaiene 91-57-6, 2-Methylnaphthalene 95-16-9, Benzothiazole 98-01-1, Furfural, biological studies 98-86-2, Acetophenone, biological studies γ -Terpinene 99-87-6, p-Cymene 100-47-0, Benzonitrile, biological 100-51-6, Benzyl alcohol, biological studies 100-52-7, studies Benzaldehyde, biological studies 100-66-3, Anisole, biological studies 104-76-7, 2-Ethylhexan-1-ol 106-21-8, 3,7-Dimethyl-1-octanol 3-Octanone 107-89-1, 3-Hydroxybutanal 107-92-6, n-Butyric acid, biological studies 107-93-7, trans-2-Butenoic acid 108-95-2, Phenol, biological studies 110-93-0, 6-Methylhept-5-en-2-one 111-27-3, 1-Hexanol, biological studies 111-71-7, Heptanal 112-05-0, Nonanoic acid 112-32-3, n-Octyl formate 112-88-9, 1-Octadecene 112-92-5, Octadecanol 118-56-9, Homomenthyl salicylate 118-60-5, 2-Ethylhexyl 119-61-9, Benzophenone, biological studies 122-00-9, salicylate p-Methylacetophenone 122-78-1, Phenyl acetaldehyde 123-35-3, Myrcene 123-42-2, 4-Hydroxy-4-methyl-2-pentanone 123-51-3, Iso-Amyl alcohol 123-72-8, Butanal 124-07-2, Octanoic acid, biological studies 124-13-0, Octanal 124-19-6, Nonanal 126-33-0, Tetrahydrothiophene, 1,1,dioxide 127-91-3, β -Pinene 128-37-0, Ionol, biological studies 137-32-6, 2-Methylbutan-1-ol 138-86-3, Limonene 142-62-1, Caproic acid, biological studies 142-91-6, Isopropyl palmitate 149-57-5, 2-Ethylhexanoic acid 289-16-7, 1,2,4-Trithiolane 291-22-5, 1,2,4,5-Tetrathiane 292-45-5, 1,2,4,6-Tetrathiepane 470-82-6, 1,8-Cineole 473-13-2, α -Selinene 483-76-1, δ -Cadinene 483-78-3, Cadalene 502-61-4, Farnesene 506-42-3, trans-9-Octadecen-1-ol 512-61-8, Santalene 513-86-0, Acetoin 514-51-2, β -Patchoulene 536-74-3, Phenylacetylene 541-85-5, 5-Methyl-3-heptanone 555-10-2, β -Phellandrene 579-07-7, 1-Phenyl-1, 2-propanedione 582-24-1, α -Hydroxyacetophenone 586-62-9, Terpinolene 589-82-2, 3-Heptanol 589-98-0, Octan-3-ol 616-25-1, Pent-1-en-3-ol 617-94-7,

```
\alpha, \alpha-Dimethylbenzenemethanol 623-36-9 624-92-0, Dimethyl
     disulfide 625-28-5, 3-Methyl butanenitrile 644-30-4, \alpha-Curcumene
     732-26-3, Tri-tert-butyl phenol 926-37-4, 4,4-Dimethylpent-2-enal
     928-96-1, cis-Hex-3-en-1-ol 930-60-9, 2-Cyclopentene-1,4-dione
     933-48-2, Trixanol 1454-85-9, 1-Heptadecanol 1576-95-0, cis-2-Pentenol
     1618-26-4, 2,4-Dithiapentane 1620-98-0,
     3,5-Di-tert-butyl-4-hydroxybenzaldehyde 1741-83-9, 2-Thiaheptane
     1795-15-9, Octylcyclohexane 1879-07-8, cis-p-Menth-8-ene 1879-09-0,
     6-\text{tert-Butyl-2}, 4-\text{dimethyl} phenol 2277-20-5, 6-\text{Nonenal}, (E) - 2314-48-9,
     Carbonotrithioic acid dimethyl ester 2436-90-0, Citronellene
     3338-55-4, cis-\beta-Ocimene 3387-41-5, Sabinene 3391-86-4,
     1-Octen-3-ol 3491-57-4 3592-19-6 3658-80-8, Dimethyl trisulfide
     3777-69-3, 2-Pentylfuran 3913-02-8, 2-Butyl octanol 4130-42-1,
     2,6-Bis(1,1-dimethylethyl)-4-ethylphenol 4170-30-3, 2-Butenal
     4312-99-6, 1-Octen-3-one 4630-07-3, Valencene 4829-04-3,
     1,3-Dithiolane 5008-72-0 5418-86-0 6540-86-9, 2,4,6-Trithiaheptane
     6617-49-8 6728-26-3, trans-Hex-2-en-1-al 6753-98-6, Humulene
     6938-51-8, 2-Octylbenzoate 10522-26-6, 2-Methyl-1-undecanol
     15193-25-6, o-Menth-8-ene 16225-26-6, 3,5-Di-tert-butylbenzoic acid
     16630-52-7, 3-Methylthiobutanal 17066-67-0, \beta-Selinene
     17283-81-7, Dihydro \beta-ionone 17699-14-8, \alpha-Cubebene 18794-84-8, Trans-\beta-Farnesene 19780-25-7, 2-Ethyl-2-butenal
                  23986-74-5, Germacrene D 27070-58-2, Octadecene
     20068-02-4
     27251-68-9, Pentadecene 27625-35-0, 3-Methylbutyl 2-methylbutyrate 33577-16-1 38514-13-5, 3-Ethyl-4-methyl-1-pentanol 38634-59-2,
     Methylthiomethyl acetyl sulfide 42474-44-2, 2,3,5-Trithiahexane
     51154-96-2, Massoialactone 58809-73-7, 2-Methylthiopropionic acid
                  66537-40-4 80466-34-8, 2,4-Hexadienal 85544-38-3,
     66537-39-1
     2,4,5,7-Tetrathiaoctane 103240-92-2 117210-66-9
                                                             119117-00-9
     415686-96-3 415687-00-2
     RL: ANT (Analyte); BSU (Biological study, unclassified); OCU (Occurrence,
     unclassified); ANST (Analytical study); BIOL (Biological study); OCCU
     (Occurrence)
        (headspace aroma of wild onion trees)
L29 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER:
                         2000:871753 HCAPLUS
```

DOCUMENT NUMBER: 134:99830

TITLE: m-Dimethoxybenzene

AUTHOR(S): Letizia, C. S.; Cocchiara, J.; Wellington, G. A.;

Funk, C.; Api, A. M.

CORPORATE SOURCE: Research Institute for Fragrance Materials, Inc.,

Hackensack, NJ, 07601, USA

SOURCE: Food and Chemical Toxicology (2000), 38(Suppl. 3),

S59-S62

CODEN: FCTOD7; ISSN: 0278-6915

Elsevier Science Ltd. PUBLISHER:

DOCUMENT TYPE: Journal English LANGUAGE:

ABSTRACT:

M-Dimethoxybenzene is approved by FDA for food use and was given Generally Recognized As Safe status as a flavor ingredient by Flavor and Extract Manufacturers' Association The Council of Europe (1992) included m-dimethoxybenzene in Category A flavoring substances, which may be used in foodstuffs.

- SO Food and Chemical Toxicology (2000), 38(Suppl. 3), S59-S62 CODEN: FCTOD7; ISSN: 0278-6915
- M-Dimethoxybenzene is approved by FDA for food use and was given Generally AB Recognized As Safe status as a flavor ingredient by Flavor and Extract Manufacturers' Association The Council of Europe (1992) included

m-dimethoxybenzene in Category A flavoring substances, which may be used in foodstuffs.

ST dimethoxybenzene flavoring food

IT Flavoring materials

(dimethoxybenzene as flavoring agent for food use)

IT 151-10-0

RL: BUU (Biological use, unclassified); FFD (Food or feed use); BIOL (Biological study); USES (Uses)

(dimethoxybenzene as flavoring agent for food use)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

SO Food and Chemical Toxicology (2000), 38(Suppl. 3), S59-S62 CODEN: FCTOD7; ISSN: 0278-6915

AB M-Dimethoxybenzene is approved by FDA for food use and was given Generally Recognized As Safe status as a flavor ingredient by Flavor and Extract Manufacturers' Association The Council of Europe (1992) included m-dimethoxybenzene in Category A flavoring substances, which may be used in foodstuffs.

ST dimethoxybenzene flavoring food

IT Flavoring materials

(dimethoxybenzene as flavoring agent for food use)

IT 151-10-0

RL: BUU (Biological use, unclassified); FFD (Food or feed use); BIOL (Biological study); USES (Uses)

(dimethoxybenzene as flavoring agent for food use)

L29 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2000:128824 HCAPLUS

DOCUMENT NUMBER: 132:149046

TITLE: The flavor composition of umbelliferous fruits. Part

1. Anise (Pimpinella anisum)

AUTHOR(S): Kollmannsberger, H.; Fricke, G.; Paulus, H.; Nitz, S. CORPORATE SOURCE: Institut fur Lebensmitteltechnologie und Analytische

Chemie, Technische Universitat Munchen, Freising,

D-85350, Germany

SOURCE: Advances in Food Sciences (2000), 22(1/2), 47-61

exts. was investigated by gaschromatog. - mass spectrometry (GC-MS) with

CODEN: AFSCF2; ISSN: 1431-7737

PUBLISHER: Advances in Food Sciences

DOCUMENT TYPE: Journal LANGUAGE: German

ABSTRACT:

Aniseed (P. anisum) was extracted with diethylether (LSM), simultaneous distillation extraction (SDE) and CO2 supercrit. fluid extraction (SFE). The flavor composition of the $\frac{1}{2}$

simultaneous effluent sniffing detection. 150 Substances (e.g. 22 monoterpenoids, 32 sesquiterpenoids, 52 phenolic or aromatic compds.) and 20 not aromatic esters could be identified. The occurrence of isomeric pseudo-isoeugenols and pseudo-isoeugenol methylethers, pseudo-isovanillyl-2-methylbutanoate, some O-containing and aromatic himachalene derivs., as well as isomeric himachalatriens could be confirmed. The most odoriferous flavor compds. were trans-anethol and ethyl-2-methylbutanoate in all exts. SFE and LSM exts. show a remarkable higher content in higher boiling components (e.g. vanillin with its strong sweet flavor). The amount of low boiling compds. is very similar in all exts. Nevertheless some odoriferous trace components like methional, phenylacetaldehyde and other thermal induced artifacts impart a typical cooking flavor note to the distillate. These differences are regarded to be responsible for the bad sensorial quality of the distillate compared to the other exts.

(Pimpinella anisum) Advances in Food Sciences (2000), 22(1/2), 47-61 SO CODEN: AFSCF2; ISSN: 1431-7737 Aniseed (P. anisum) was extracted with diethylether (LSM), simultaneous distillation extraction (SDE) and CO2 supercrit. fluid extraction (SFE). The flavor composition of the exts. was investigated by qaschromatog. - mass spectrometry (GC-MS) with simultaneous effluent sniffing detection. 150 Substances (e.g.. . . pseudo-isoeugenol methylethers, pseudo-isovanillyl-2-methylbutanoate, some O-containing and aromatic himachalene derivs., as well as isomeric himachalatriens could be confirmed. The most odoriferous flavor compds. were trans-anethol and ethyl-2-methylbutanoate in all exts. SFE and LSM exts. show a remarkable higher content in higher boiling components (e.g. vanillin with its strong sweet flavor). The amount of low boiling compds. is very similar in all exts. Nevertheless some odoriferous trace components like methional, phenylacetaldehyde and other thermal induced artifacts impart a typical cooking flavor note to the distillate. These differences are regarded to be responsible for the bad sensorial quality of the distillate compared. ST Anise seed flavor essential oil volatile GCMS; Pimpinella seed flavor essential oil volatile GCMS ΙT Anise Flavor Volatile substances (flavor composition of Pimpinella anisum determined by GC/MS) ΙT Essential oils Monoterpenes Sesquiterpenes RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence) (flavor composition of Pimpinella anisum determined by GC/MS) TТ 60-12-8, Phenyl ethanol 66-25-1, Hexanal 76-22-2, Camphor 78-70-6, Linalool 79-77-6, β -Ionone 79-92-5, Camphene 80-56-8, α -Pinene 89-80-5, Menthone 90-02-8, 2-Hydroxy-benzaldehyde, biological studies 90-05-1, Guaiacol 93-02-7, 2,5-Dimethoxy-benzaldehyde 94-30-4, Ethyl anisate 98-01-1, Furfural, biological studies 98-55-5, α -Terpineol 99-49-0, Carvone 99-87-6, p-Cymene 100-06-1 100-09-4, 99-85-4, γ -Terpinene p-Methoxy benzoic acid 100-42-5, Styrol, biological studies Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological 100-66-3, Anisol, biological studies 104-45-0 104-46-1D, Anethol, dimers 105-13-5, Anisic alcohol 111-27-3, Hexanol, biological studies 111-61-5, Ethyl octadecanoate 112-39-0, Methyl 112-61-8, Methyl octadecanoate 116-53-0, 2-Methyl hexadecanoate 121-33-5, Vanillin 121-97-1 122-00-9, 121-98-2 butyric acid p-Methylacetophenone 122-78-1, Phenylacetaldehyde 122-84-9 123-11-5. Anis aldehyde, biological studies 123-11-5D, Anisaldehyde, dimer, biological studies 123-35-3, Myrcene 124-06-1, Ethyl tetradecanoate 124-10-7, Methyl tetradecanoate 124-13-0, Octanal 127-91-3, β-Pinene 138-86-3, Limonene 140-67-0, Methylchavicol 142-62-1, Hexanoic acid, biological studies 150-76-5, p-Methoxyphenol 301-00-8 470-82-6, 1,,8-Cineol 483-76-1, δ -Cadinene Phytol 491-07-6, Iso-menthone 483-77-2, Calamenene 483-78-3, Cadalene

495-60-3, α -Zingiberene 495-61-4, β -Bisabolene 502-69-2

Borneol 515-13-9, β -Elemene 546-80-5, Thujone 562-74-3

584-82-7

503-74-2, 3-Methyl butyric acid 504-96-1, Neophytadiene 507-70-0,

644-30-4 673-22-3 868-57-5, Methyl-2-methylbutanoate 928-68-7 1003-29-8, 2-Formyl pyrrole 1072-83-9, 2-Acetyl pyrrole 1137-12-8,

585-25-1, 2,3-Octanedione 628-97-7, Ethyl hexadecanoate

```
2436-90-0, \beta-Citronellene 2445-67-2, Isobutyl-2-methylbutanoate
    2445-78-5, 2-Methylbutyl-2-methylbutanoate 2777-58-4
                                                             3268-49-3,
    Methional 3319-15-1 3380-68-5 3387-41-5, Sabinene 3853-83-6,
                   3856-25-5, \alpha-Copaene
                                           4180-23-8,
    \alpha-Himachalene
    trans-Anethol
                    4312-99-6, 1-Octen-3-one
                                              5025-38-7
                                                           5349-60-0
    5975-49-5, Isogeijerene 5989-08-2, \alpha-Longipinene 6728-26-3
    6750-60-3, Spathulenol 6902-73-4D, Geijerene, derivs. 7132-64-1,
    Methyl pentadecanoate 7370-44-7, 5-Hexadecanolide 7452-79-1,
    Ethyl-2-methylbutanoate 7784-99-8, Vinylquaiacol
                                                       10032-15-2,
    Hexyl-2-methylbutanoate 13391-27-0 13474-59-4
                                                       14912-44-8,
                 17627-44-0, \alpha-Bisabolene 18794-84-8
    α-Ylangene
    18829-56-6
                19419-67-1, ar-Himachalene 19754-22-4
                                                         19785-01-4
    19785-02-5 20307-83-9, \beta-Sesquiphellandrene 20307-84-0,
    \delta-Elemene 21391-99-1, \alpha-Calacorene
                                          23726-93-4,
                   25679-28-1 27625-35-0,
    β-Damascenone
    3-Methylbutyl-2-methylbutanoate 27739-28-2 28061-47-4 29960-49-4
    30314-64-8 34302-52-8 41587-31-9, Vinylanisole
                                                         50277-34-4,
    \beta-Calacorene 51766-65-5 53111-25-4, \gamma-Himachalene
    56144-27-5 58989-20-1 60026-20-2 60784-31-8 64825-84-9
                 71672-25-8, Ethyl octadecadienoate 78204-62-3
    64825-85-0
                                                                  78446-77-2
    88395-46-4, Iso-spathulenol 97180-28-4 98755-19-2 98755-22-7
                               121198-16-1, Ethyl octadecatrienoate
    106871-14-1
                 115569-82-9
    150133-25-8
                  227960-21-6, Himachal-2-en-6-ol 257887-98-2
                                                                 257888-07-6
    257888-10-1
                  257888-13-4
                                257888-15-6
    RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study,
    unclassified); ANST (Analytical study); BIOL (Biological study); OCCU
     (Occurrence)
        (flavor composition of Pimpinella anisum determined by GC/MS)
OS.CITING REF COUNT:
                        7
                              THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
                               (7 CITINGS)
                              THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                        65
                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
    The flavor composition of umbelliferous fruits. Part 1. Anise
ΤI
     (Pimpinella anisum)
SO
    Advances in Food Sciences (2000), 22(1/2), 47-61
    CODEN: AFSCF2; ISSN: 1431-7737
    Aniseed (P. anisum) was extracted with diethylether (LSM), simultaneous
distillation
    extraction (SDE) and CO2 supercrit. fluid extraction (SFE). The flavor
composition of
    the exts. was investigated by gaschromatog. - mass spectrometry (GC-MS)
    with simultaneous effluent sniffing detection. 150 Substances (e.g. 22
    monoterpenoids, 32 sesquiterpenoids, 52 phenolic or aromatic compds.) and 20
    not aromatic esters could be identified. The occurrence of isomeric
    pseudo-isoeugenols and pseudo-isoeugenol methylethers,
    pseudo-isovanillyl-2-methylbutanoate, some O-containing and aromatic
himachalene
    derivs., as well as isomeric himachalatriens could be confirmed. The most
    odoriferous flavor compds. were trans-anethol and
    ethyl-2-methylbutanoate in all exts. SFE and LSM exts. show a remarkable
    higher content in higher boiling components (e.g. vanillin with its strong
    sweet flavor). The amount of low boiling compds. is very similar in all
    exts. Nevertheless some odoriferous trace components like methional,
    phenylacetaldehyde and other thermal induced artifacts impart a typical
    cooking flavor note to the distillate. These differences are regarded
    to be responsible for the bad sensorial quality of the distillate compared
    to the other exts.
    Anise seed flavor essential oil volatile GCMS; Pimpinella seed flavor
ST
    essential oil volatile GCMS
```

Anise

ΤТ

Longicyclene 1195-79-5, Fenchone 1461-03-6, β -Himachalene

Volatile substances (flavor composition of Pimpinella anisum determined by GC/MS) ΙT Essential oils Monoterpenes Sesquiterpenes RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence) (flavor composition of Pimpinella anisum determined by GC/MS) 60-12-8, Phenyl ethanol 66-25-1, Hexanal 76-22-2, Camphor ΤТ 79-77-6, β -Ionone 79-92-5, Camphene 80-56-8, Linalool α -Pinene 89-80-5, Menthone 90-02-8, 2-Hydroxy-benzaldehyde, biological studies 90-05-1, Guaiacol 93-02-7, 2,5-Dimethoxy-benzaldehyde 94-30-4, Ethyl anisate 98-01-1, Furfural, biological studies 98-55-5, α -Terpineol 99-49-0, Carvone 99-85-4, γ -Terpinene 99-87-6, p-Cymene 100-06-1 100-09-4, p-Methoxy benzoic acid 100-42-5, Styrol, biological studies 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 100-66-3, Anisol, biological studies 104-45-0 104-46-1D, Anethol, dimers 105-13-5, Anisic alcohol 111-27-3, Hexanol, biological studies 111-61-5, Ethyl octadecanoate 112-39-0, Methyl 112-61-8, Methyl octadecanoate 116-53-0, 2-Methyl hexadecanoate 121-33-5, Vanillin 121-97-1 butyric acid 121-98-2 122-00-9, 122-78-1, Phenylacetaldehyde 122-84-9 123-11-5, p-Methylacetophenone Anis aldehyde, biological studies 123-11-5D, Anisaldehyde, dimer, biological studies 123-35-3, Myrcene 124-06-1, Ethyl tetradecanoate 124-10-7, Methyl tetradecanoate 124-13-0, Octanal 127-91-3, β -Pinene 138-86-3, Limonene 140-67-0, Methylchavicol 142-62-1, Hexanoic acid, biological studies 150-76-5, p-Methoxyphenol 150 - 86 - 7, Phytol 301-00-8 470-82-6, 1,,8-Cineol 483-76-1, δ -Cadinene 483-77-2, Calamenene 483-78-3, Cadalene 491-07-6, Iso-menthone 495-60-3, α -Zingiberene 495-61-4, β -Bisabolene 502-69-2 503-74-2, 3-Methyl butyric acid 504-96-1, Neophytadiene 507-70-0, 515-13-9, β -Elemene 546-80-5, Thujone 562-74-3 Borneol 584-82-7 585-25-1, 2,3-Octanedione 628-97-7, Ethyl hexadecanoate 673-22-3 868-57-5, Methyl-2-methylbutanoate 644-30-4 928-68-7 1003-29-8, 2-Formyl pyrrole 1072-83-9, 2-Acetyl pyrrole Longicyclene 1195-79-5, Fenchone 1461-03-6, β -Himachalene 2436-90-0, β -Citronellene 2445-67-2, Isobutyl-2-methylbutanoate 2445-78-5, 2-Methylbutyl-2-methylbutanoate 2777-58-4 Methional 3319-15-1 3380-68-5 3387-41-5, Sabinene 3853-83-6, α -Himachalene 3856-25-5, α -Copaene 4180-23-8, trans-Anethol 4312-99-6, 1-Octen-3-one 5025-38-7 5349-60-0 5975-49-5, Isogeijerene 5989-08-2, α -Longipinene 6728-26-3 6750-60-3, Spathulenol 6902-73-4D, Geijerene, derivs. 7132-64-1, Methyl pentadecanoate 7370-44-7, 5-Hexadecanolide 7452-79-1, Ethyl-2-methylbutanoate 7784-99-8, Vinylguaiacol 10032-15-2, Hexyl-2-methylbutanoate 13391-27-0 13474-59-4 14912-44-8, 17627-44-0, α -Bisabolene 18794-84-8 α-Ylangene 19419-67-1, ar-Himachalene 19754-22-4 1978 20307-83-9, β -Sesquiphellandrene 20307-84-0, 18829-56-6 19785-01-4 19785-02-5 21391-99-1, α -Calacorene 23726-93-4, δ -Elemene 25679-28-1 27625-35-0, β-Damascenone 3-Methylbutyl-2-methylbutanoate 27739-28-2 28061-47-4 34302-52-8 41587-31-9, Vinylanisole 30314-64-8 50277-34-4, β-Calacorene 51766-65-5 53111-25-4, γ -Himachalene $56144-27-5 \qquad 58989-20-1 \qquad 60026-20-2 \qquad 60784-31-8 \qquad 64825-84-9$ 71672-25-8, Ethyl octadecadienoate 78204-62-3 78446-77-2 64825-85-0 88395-46-4, Iso-spathulenol 97180-28-4 98755-19-2 98755-22-7 106871-14-1 115569-82-9 121198-16-1, Ethyl octadecatrienoate

Flavor

150133-25-8 227960-21-6, Himachal-2-en-6-ol 257887-98-2 257888-07-6

257888-10-1 257888-13-4 257888-15-6

RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence)

(flavor composition of Pimpinella anisum determined by GC/MS)

L29 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1998:256643 HCAPLUS

DOCUMENT NUMBER: 128:243078

ORIGINAL REFERENCE NO.: 128:48133a,48136a

New Components with Potential Antioxidant and

Organoleptic Properties, Detected for the First Time

in Liquid Smoke Flavoring Preparations Guillen, Maria D.; Ibargoitia, Maria L.

AUTHOR(S): CORPORATE SOURCE: Tecnologia de Alimentos Facultad de Farmacia,

Universidad del Pais Vasco, Vitoria, 01006, Spain Journal of Agricultural and Food Chemistry (1998),

46(4), 1276-1285

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

ABSTRACT:

SOURCE:

A com. aqueous smoke preparation was exhaustively extracted, using dichloromethane

solvent, until the carrier had totally lost its smoky odor. Qual. and quant. characterizations of the extract were performed by means of gas chromatog./mass spectrometry and gas chromatog. with flame ionization detector, resp. Carbonyl derivs. including aldehydes and ketones as well as acids and esters are almost absent; however, the high proportion of phenol, guaiacol, and syringol derivs. is noticeable. The presence of di-tert-butylhydroxytoluene, several hopanes, and a number of lignin dimers must be pointed out; these latter components had apparently not been detected before either in smoke flavorings or in wood smoke. The mass spectral data of the compds. considered as lignin dimers and of the unidentified components are given. The presence of lignin dimers is very interesting from the point of view of health and food technol. for their therapeutic, organoleptic, and antioxidant properties.

- New Components with Potential Antioxidant and Organoleptic Properties, Detected for the First Time in Liquid Smoke Flavoring Preparations
- SO Journal of Agricultural and Food Chemistry (1998), 46(4), 1276-1285 CODEN: JAFCAU; ISSN: 0021-8561
- AR . . . number of lignin dimers must be pointed out; these latter components had apparently not been detected before either in smoke flavorings or in wood smoke. The mass spectral data of the compds. considered as lignin dimers and of the unidentified components. . .
- smoke flavoring compn ST
- Alcohols, biological studies

Aldehydes, biological studies

Aromatic hydrocarbons, biological studies

Ethers, biological studies Ketones, biological studies Phenols, biological studies Terpenes, biological studies

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

ΙT Triterpenes RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(hopane; components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

IT Flavoring materials

(smoke flavors; components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

ΙT 60-12-8, 2-Phenylethanol 64-19-7, Acetic acid, biological studies 67-64-1, 2-Propanone, biological studies 75-07-0, Acetaldehyde, biological studies 78-93-3, 2-Butanone, biological studies 85-01-8, Phenanthrene, biological studies 88-18-6, 2-(1,1-Dimethylethyl)phenol 89-83-8, Thymol 90-00-6, 2-Ethylphenol 90-05-1, Guaiacol 91-10-1, Syringol 91-16-7 91-20-3, Naphthalene, biological studies 93-15-2 93-16-3 93-51-6, 4-Methylguaiacol 95-48-7, 2-Methylphenol, biological 95-87-4, 2,5-Dimethylphenol 97-53-0, Eugenol 98-00-0, studies Furfuryl alcohol 98-86-2, Acetophenone, biological studies 99-49-0, Carvone 99-87-6, p-Cymene 100-42-5, biological studies 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 102-25-0, 1,3,5-Triethylbenzene 104-87-0, 4-Methylbenzaldehyde 105-67-9, 2,4-Dimethylphenol 106-44-5, biological studies 108-39-4, biological studies 118-68-9, 3,5-Dimethylphenol 108-95-2, Phenol, biological studies 111-02-4, Squalene 112-95-8, Eicosane 121-33-5, Vanillin 121-34-6, Vanillic acid 134-96-3, Syringaldehyde 140-67-0, 150-78-7, 1,4-Dimethoxybenzene 151-10-0, Estragole 1,3-Dimethoxybenzene 458-35-5, Coniferyl alcohol 470-82-6, Eucalyptol 487-11-6, 5-(2-Propenyl)-1,2,3-trimethoxybenzene 487-12-7 494-99-5, 3,4-Dimethoxytoluene 496-78-6, 2,4,5-Trimethylphenol 498-02-2, Acetovanillone 499-75-2, Carvacrol 526-75-0, 2,3-Dimethylphenol 526-85-2, 2,3,4-Trimethylphenol 527-60-6, 2,4,6-Trimethylphenol 539-12-8, 4-Propenylphenol 544-76-3, Hexadecane 544-85-4**,** Dotriacontane 576-26-1 577-16-2, 1-(2-Methylphenyl)ethanone 585-34-2, 3-(1,1-Dimethylethyl)phenol 593-45-3, Octadecane 593-49-7, Heptacosane 620-17-7, 3-Ethylphenol 629-59-4, Tetradecane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 629-99-2, Pentacosane 630-01-3, Hexacosane 630-02-4, Octacosane 630-03-5, Nonacosane 630-04-6, Hentriacontane 630-05-7, 634-36-6, 1,2,3-Trimethoxybenzene 638-67-5, Tricosane Tritriacontane 638-68-6, Triacontane 644-35-9, 2-Propylphenol 645-56-7, 4-Propylphenol 646-31-1, Tetracosane 697-82-5, 2,3,5-Trimethylphenol 698-71-5, 3-Ethyl-5-methylphenol 705-15-7 719-22-2, 2,6-Bis(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione 832-69-9, 944-99-0, 2,6-Dimethoxyphenyl acetate 1121-05-7 1-Methylphenanthrene 1123-94-0, 4-Ethyl-3-methylphenol 1136-86-3 1192-62-7 1620-98-0, 4-Hydroxy-3,5-di-tert-butylbenzaldehyde 1655-68-1 2033-89-8, 3,4-Dimethoxyphenol 2416-94-6 2478-38-8, 1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone 2503-46-0 2758-18-1 2785-87-7, 4-Propylquaiacol 2785-89-9, 4-Ethylquaiacol 3194-15-8 3840-31-1 5779-72-6, 2,4,5-Trimethylbenzaldehyde 5912-86-7, cis-Isoeugenol 5932-68-3, trans-Isoeugenol 6004-60-0 6627-88-9 6635-22-9 6638-05-7, 4-Methylsyringol 6766-82-1, 4-Propylsyringol 7786-61-0, 4-Vinylguaiacol 13849-96-2, $17\alpha(H)$, $21\beta(H)$ -Hopane 14059-92-8, 4-Ethylsyringol 14167-59-0, Tetratriacontane 18435-45-5, 18435-54-6, 1-Hentriacontene 20983-15-7 24810-59-1 1-Nonadecene 26998-80-1, Trimethylphenol 27587-17-3, 2-Methyl-1, 4-benzenedicarboxaldehyde 28343-22-8, 4-Vinylsyringol 28777-87-9, Hydroxybenzaldehyde 28790-86-5, 2,3,4-Trimethy1-2-cyclopenten-1-one 30434-65-2 32556-65-3 39831-51-1 53584-62-6, Homohopane 53951-50-1, Ethylbenzaldehyde 54311-28-3,

55683-21-1, 3,4,5-Trimethyl-2-cyclopenten-1-oneBishomohopane 59893-87-7 60553-44-8 61868-12-0, 1-Tetratriacontene 66309-82-8 69271-91-6 71629-80-6, Trishomohopane 71880-75-6 79755-53-6 82000-05-3 120550-70-1 204781-71-5 81825-21-0 204781-72-6, A'-Neo-28-norgammacerane 204781-73-7 204781-74-8 RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

OS.CITING REF COUNT: 50 THERE ARE 50 CAPLUS RECORDS THAT CITE THIS RECORD (51 CITINGS)

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

- TI New Components with Potential Antioxidant and Organoleptic Properties, Detected for the First Time in Liquid Smoke Flavoring Preparations
- SO Journal of Agricultural and Food Chemistry (1998), 46(4), 1276-1285 CODEN: JAFCAU; ISSN: 0021-8561
- ${\tt AB}$ A com. aqueous smoke preparation was exhaustively extracted, using dichloromethane as

solvent, until the carrier had totally lost its smoky odor. Qual. and quant. characterizations of the extract were performed by means of gas chromatog./mass spectrometry and gas chromatog. with flame ionization detector, resp. Carbonyl derivs. including aldehydes and ketones as well as acids and esters are almost absent; however, the high proportion of phenol, guaiacol, and syringol derivs. is noticeable. The presence of di-tert-butylhydroxytoluene, several hopanes, and a number of lignin dimers must be pointed out; these latter components had apparently not been detected before either in smoke flavorings or in wood smoke. The mass spectral data of the compds. considered as lignin dimers and of the unidentified components are given. The presence of lignin dimers is very interesting from the point of view of health and food technol. for their therapeutic, organoleptic, and antioxidant properties.

ST smoke flavoring compn

IT Alcohols, biological studies
Aldehydes, biological studies
Aromatic hydrocarbons, biological studies
Ethers, biological studies
Ketones, biological studies
Phenols, biological studies
Terpenes, biological studies
RL: BAC (Biological activity or effector.

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

IT Triterpenes

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(hopane; components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

IT Flavoring materials

(smoke flavors; components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

IT 60-12-8, 2-Phenylethanol 64-19-7, Acetic acid, biological studies 67-64-1, 2-Propanone, biological studies 75-07-0, Acetaldehyde, biological studies 78-93-3, 2-Butanone, biological studies 85-01-8, Phenanthrene, biological studies 88-18-6, 2-(1,1-Dimethylethyl)phenol

89-83-8, Thymol 90-00-6, 2-Ethylphenol 90-05-1, Guaiacol 91-10-1, Syringol 91-16-7 91-20-3, Naphthalene, biological studies 93-15-2 93-16-3 93-51-6, 4-Methylguaiacol 95-48-7, 2-Methylphenol, biological studies 95-87-4, 2,5-Dimethylphenol 97-53-0, Eugenol 98-00-0, Furfuryl alcohol 98-86-2, Acetophenone, biological studies 99-49-0, Carvone 99-87-6, p-Cymene 100-42-5, biological studies 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 102-25-0, 1,3,5-Triethylbenzene 104-87-0, 4-Methylbenzaldehyde 105-67-9, 2,4-Dimethylphenol 106-44-5, biological studies 108-39-4, biological studies 108-68-9, 3,5-Dimethylphenol 108-95-2, Phenol, biological studies 111-02-4, Squalene 112-95-8, Eicosane 121-33-5, Vanillin 121-34-6, Vanillic acid 134-96-3, Syringaldehyde 140-67-0, Estragole 150-78-7, 1,4-Dimethoxybenzene 151-10-0, 1,3-Dimethoxybenzene 458-35-5, Coniferyl alcohol 470-82-6, Eucalyptol 487-11-6, 5-(2-Propenyl)-1,2,3-trimethoxybenzene 487-12-7 494-99-5, 3,4-Dimethoxytoluene 496-78-6, 2,4,5-Trimethylphenol 498-02-2, Acetovanillone 499-75-2, Carvacrol 526-75-0, 2,3-Dimethylphenol 526-85-2, 2,3,4-Trimethylphenol 527-60-6, 2,4,6-Trimethylphenol 539-12-8, 4-Propenylphenol 544-76-3, Hexadecane 544-85-4, Dotriacontane 576-26-1 577-16-2, 1-(2-Methylphenyl)ethanone585-34-2, 3-(1,1-Dimethylethyl)phenol 593-45-3, Octadecane 593-49-7, Heptacosane 620-17-7, 3-Ethylphenol 629-59-4, Tetradecane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 629-99-2, Pentacosane 630-01-3, Hexacosane 630-02-4, Octacosane 630-03-5, Nonacosane 630-04-6, Hentriacontane 630-05-7, Tritriacontane 634-36-6, 1,2,3-Trimethoxybenzene 638-67-5, Tricosane 638-68-6, Triacontane 644-35-9, 2-Propylphenol 645-56-7, 4-Propylphenol 646-31-1, Tetracosane 697-82-5, 2,3,5-Trimethylphenol 698-71-5, 3-Ethyl-5-methylphenol 705-15-7 719-22-2, 2,6-Bis(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione 832-69-9, 1-Methylphenanthrene 944-99-0, 2,6-Dimethoxyphenyl acetate 1121-05-7 1123-94-0, 4-Ethyl-3-methylphenol 1136-86-3 1192-62-7 1620-98-0, 4-Hydroxy-3,5-di-tert-butylbenzaldehyde 1655-68-1 2033-89-8, 3,4-Dimethoxyphenol 2416-94-6 2478-38-8, 1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone 2503-46-0 2758-18-1 2785-87-7, 4-Propylguaiacol 2785-89-9, 4-Ethylguaiacol 3194-15-8 3840-31-1 5779-72-6, 2,4,5-Trimethylbenzaldehyde 5912-86-7, cis-Isoeugenol 5932-68-3, trans-Isoeugenol 6004-60-0 6638-05-7, 4-Methylsyringol 6766-82-1, 4-Propylsyringol 6635-22-9 7786-61-0, 4-Vinylguaiacol 13849-96-2, $17\alpha(H)$, $21\beta(H)$ -Hopane 14059-92-8, 4-Ethylsyringol 14167-59-0, Tetratriacontane 18435-45-5, 1-Nonadecene 18435-54-6, 1-Hentriacontene 20983-15-7 24810-59-1 26998-80-1, Trimethylphenol 27587-17-3, 2-Methyl-1, 4-benzenedicarboxaldehyde 28343-22-8, 4-Vinylsyringol 28777-87-9, Hydroxybenzaldehyde 28790-86-5, 2,3,4-Trimethyl-2-cyclopenten-1-one 30434-65-2 32556-65-3 39831-51-1 53584-62-6, Homohopane 53951-50-1, Ethylbenzaldehyde 54311-28-3, Bishomohopane 55683-21-1, 3,4,5-Trimethyl-2-cyclopenten-1-one 59893-87-7 60553-44-8 61868-12-0, 1-Tetratriacontene 66309-82-8 71629-80-6, Trishomohopane 71880-75-6 79755-53-6 69271-91-6 81825-21-0 82000-05-3 120550-70-1 204781-71-5 A'-Neo-28-norgammacerane 204781-73-7 204781-74-8 204781-72-6, RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (components with potential antioxidant and organoleptic properties,

L29 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN ACCESSION NUMBER: 1997:94109 HCAPLUS Correction of: 1996:449693

detected for the first time in liquid smoke flavoring)

DOCUMENT NUMBER: 126:108688

Correction of: 125:95620

ORIGINAL REFERENCE NO.: 126:20923a

TITLE: Antiplaque, antigingivitis oral compositions

containing phosphates and copper sources Sanker, Lowell Alan; Upson, James Grigg

PATENT ASSIGNEE(S): Procter and Gamble Company, USA

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

INVENTOR(S):

PA'	TENT :	NO.			KIN	D	DATE			APPL	ICAT	I NOI	. O <i>V</i>		D	ATE	
WO	9615	 768			A1	_	 1996	0530	,	WO 1	 995-1	 US140	013		1	9951	 027 <
	W:	ΑM,	ΑU,	BB,	BG,	BR,	BY,	CA,	CN,	CZ,	EE,	FΙ,	GE,	HU,	IS,	JP,	KG,
		KP,	KR,	KΖ,	LK,	LR,	LT,	LV,	MD,	MG,	MK,	MN,	MX,	NO,	NZ,	PL,	RO,
		RU,	SG,	SI,	SK,	ТJ,	TM,	TT,	UA,	UZ,	VN						
	RW:	KΕ,	LS,	MW,	SD,	SZ,	UG,	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,
		IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML,	MR,
		ΝE,	SN,	TD,	ΤG												
AU	9540	160			Α		1996	0617		AU 1	995-	40160	0		1	9951	027 <
IN	1995	DE02	032		Α		2005	0311		IN 1	995-	DE203	32		1	9951	106
US	5628	986			Α		1997	0513		US 1	996-	63293	36		1	9960	416 <
PRIORIT	Y APP	LN.	INFO	.:						US 1	994-	3417	16	ž	A 1	9941	118
									,	WO 1	995-1	US140	013	Ī	W 1	9951)27

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT ABSTRACT:

Disclosed are oral compns. such as toothpastes, mouth rinses, lozenges, and gums containing at least one phosphate derivative and a copper source. A mouthwash contained water 70.86, sorbitol solution (70 %) 10.25, Na saccharin 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl monophosphate 0.35 %.

```
PΙ
    WO 9615768 A1 19960530
    PATENT NO.
                      KIND DATE APPLICATION NO. DATE
                       ____
                              _____
    WO 9615768
                       A1 19960530 WO 1995-US14013 19951027 <--
PΙ
        W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG,
            KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO,
            RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN
        RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE,
            IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR,
            NE, SN, TD, TG
    AU 9540160
                              19960617
                                        AU 1995-40160
                                                                19951027 <--
                       Α
    IN 1995DE02032
                       Α
                              20050311
                                         IN 1995-DE2032
                                                               19951106
    US 5628986
                             19970513 US 1996-632936 19960416 <--
                       Α
    . . 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl
AB
    sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor
    0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl
    monophosphate 0.35 %.
                                     89-78-1
    60-12-8, Benzeneethanol
                            78-70-6
                                               89-80-5
                                                          89-83-8
    100-52-7, Benzaldehyde, biological studies 104-45-0
                                                         104-46-1
    104-55-2 105-54-4 121-32-4 121-33-5 123-92-2 127-41-3 140-67-0 470-82-6 4422-70-2 4940-11-8 6485-40-1
                                                                    138-86-3
    RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
     (Uses)
       (as flavoring agent; antiplaque, antigingivitis dentifrices
```

containing phosphates and copper sources)
OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

PATENT NO. KIND DATE APPLICATION NO. DATE _____ ____ _____ A1 19960530 WO 1995-US14013 19951027 <--WO 9615768 PΙ W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG AU 9540160 19960617 AU 1995-40160 Α 19951027 <--IN 1995DE02032 IN 1995-DE2032 Α 20050311 19951106 US 1996-632936 US 5628986 A 19970513 19960416 <--

AB Disclosed are oral compns. such as toothpastes, mouth rinses, lozenges, and gums containing at least one phosphate derivative and a copper source. A mouthwash contained water 70.86, sorbitol solution (70 %) 10.25, Na saccharin 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl monophosphate 0.35 %.

IT 60-12-8, Benzeneethanol 78-70-6 89-78-1 89-80-5 89-83-8 97-53-0 100-52-7, Benzaldehyde, biological studies 104-45-0 104-46-1 104-55-2 105-54-4 121-32-4 121-33-5 123-92-2 127-41-3 138-86-3 140-67-0 470-82-6 4422-70-2 4940-11-8 6485-40-1 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(as flavoring agent; antiplaque, antigingivitis dentifrices containing phosphates and copper sources)

L29 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1996:449693 HCAPLUS

DOCUMENT NUMBER: 125:95620

WO 9615768 A1 19960530

PΙ

ORIGINAL REFERENCE NO.: 125:17815a,17818a

TITLE: Antiplaque, antigingivitis oral compositions

containing phosphates and copper sources INVENTOR(S): Sanker, Lowell Alan; Upson, James Grigg

PATENT ASSIGNEE(S): Procter and Gamble Company, USA

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

PATENT INFORMATION:

PAT	ENT I	NO.			KIN	D	DATE		Ž	APPL	ICAT	ION	NO.		D	ATE		
						_			-									
WO !	9615	768	A1				1996	0530	WO	199	5-US	1401	3		199.	5102	7	
W:	AM,	ΑU,	BB,	BG,	BR,	BY,	CA,	CN,	CZ,	EE,	FΙ,	GE,	HU,	IS,	JP,	KG,	KP,	
	KR,	KΖ,	LK,	LR,	LT,	LV,	MD,	MG,	MK,	MN,	MX,	NO,	NZ,	PL,	RO,	RU,	SG,	
	SI,	SK,	ΤJ,	TM,	TT,	UA,	UZ,	VN										
RW:	ΑT,	BE,	BF,	ВJ,	CF,	CG,	CH,	CI,	CM,	DE,	DK,	ES,	FR,	GΑ,	GB,	GR,	IE,	
	ΙΤ,	LU,	MC,	ML,	MR,	ΝE,	NL,	PT,	SE,	SN,	TD,	TG						
PRIORITY	APP:	LN.	INFO	.:					U:	5 19	94-3	4171	6		1	9941:	118	
ABSTRACT																		

Disclosed are oral compns. such as toothpastes, mouthrinses, lozenges, and gums containing at least one phosphate derivative and a copper source. A mouthwash contained water 70.86, sorbitol solution (70 %) 10.25, Na saccharin 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl

monophosphate 0.15, and vanilly1 monophosphate 0.35 %.

```
WO 9615768 A1 19960530
PΙ
    . . 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl
AΒ
     sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor
     0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl
     monophosphate 0.35 %.
     60-12-8, Phenylethyl alcohol 78-70-6, Linalool 89-78-1, Menthol
ΙT
     89-80-5, Menthone 89-83-8, Thymol 97-53-0, Eugenol 100-52-7,
     Benzaldehyde, biological studies 104-45-0, Dihydroanethole
     104-46-1, Anethole 104-55-2, Cinnamic aldehyde 105-54-4, Ethyl
     butyrate 121-32-4, Ethyl vanillin
                                         121-33-5, Vanillin
     Isoamyl acetate 127-41-3, \alpha-Ionone 138-86-3, Limonene
     140-67-0, Estragole 470-82-6, Eucalyptol
                                                4422-70-2
                                                            4940-11-8,
     Ethylmaltol 6485-40-1
     RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
     (Uses)
        (as flavoring agent; antiplaque, antigingivitis dentifrices
        containing phosphates and copper sources)
     WO 9615768 A1 19960530
PΤ
AΒ
     Disclosed are oral compns. such as toothpastes, mouthrinses, lozenges, and
     gums containing at least one phosphate derivative and a copper source. A
     mouthwash contained water 70.86, sorbitol solution (70 %) 10.25, Na saccharin
     0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate
     solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor 0.24,
     glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl monophosphate 0.35
ΙT
     60-12-8, Phenylethyl alcohol 78-70-6, Linalool
                                                       89-78-1, Menthol
                       89-83-8, Thymol 97-53-0, Eugenol
     89-80-5, Menthone
                                                            100-52-7,
     Benzaldehyde, biological studies 104-45-0, Dihydroanethole
     104-46-1, Anethole 104-55-2, Cinnamic aldehyde 105-54-4, Ethyl
     butyrate 121-32-4, Ethyl vanillin 121-33-5, Vanillin
                                                               123-92-2,
     Isoamyl acetate 127-41-3, \alpha-Ionone 138-86-3, Limonene
                         470-82-6, Eucalyptol
                                                4422-70-2
     140-67-0, Estragole
                                                            4940-11-8,
     Ethylmaltol
                  6485-40-1
     RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
     (Uses)
        (as flavoring agent; antiplaque, antigingivitis dentifrices
        containing phosphates and copper sources)
L29 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER:
                        1992:104811 HCAPLUS
DOCUMENT NUMBER:
                        116:104811
ORIGINAL REFERENCE NO.: 116:17729a,17732a
                        The composition of woodruff volatiles (Galium
TITLE:
                         odoratum)
                        Woerner, Martin; Schreier, Peter
AUTHOR(S):
CORPORATE SOURCE:
                        Univ. Wuerzburg, Wuerzburg, W-8700, Germany
                        Zeitschrift fuer Lebensmittel-Untersuchung und
SOURCE:
                        -Forschung (1991), 193(4), 317-20
                        CODEN: ZLUFAR; ISSN: 0044-3026
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                        German
ABSTRACT:
Studies of the composition of an aroma extract of dried woodruff by medium-pressure
liquid chromatog. following Soxhlet extraction and chlorophylls removal by
gel-permeation chromatog. revealed the presence of 225 substances, 69 of which
were alcs., 69 carbonyl compds., 22 hydrocarbons, 20 acids, 19 esters, 14
lactones and 12 other compds. Of the \gamma\text{--lactones}\text{,} multi-dimensional gas
chromatog. indicated an enantiomeric excess of the R-isomer with increasing
chain length. Only 1 substance was previously unknown in nature:
```

7,11,15-trimethyl-2-hexadecanone; it is thus proposed as an anal. indicator for the detection of the illegal use of woodruff aromas in foods.

- Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung (1991), SO 193(4), 317-20 CODEN: ZLUFAR; ISSN: 0044-3026
- ST woodruff flavor volatile
- ΙT Flavor

(woodruff, composition of)

ΙT 57-10-3, Hexadecanoic acid, biological studies 57-11-4, Octadecanoic acid, biological studies 60-12-8, 2-Phenylethanol 64-19-7, Acetic acid, biological studies 65-85-0, Benzoic acid, biological studies 66-25-1, Hexanal 71-36-3, 1-Butanol, biological studies 71-41-0, 1-Pentanol, biological studies 76-22-2 76-49-3, Bornyl acetate 78-36-4 78-70-6, Linalool 78-83-1, 2-Methyl-1-propanol, biological 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological studies studies 79-77-6, β -Ionone 79-92-5, Camphene 89-80-5, Menthone 89-81-6, Piperitone 89-82-7, Pulegone 89-83-8, Thymol 90-00-6, 2-Ethylphenol 91-64-5, Coumarin 93-15-2, Eugenylmethyl ether 93-55-0, 1-Phenylpropan-1-one 95-48-7, biological studies 98-55-5, α -Terpineol 99-49-0, Carvone 99-50-3, 3,4-Dihydroxybenzoic acid 99-85-4, γ-Terpinen 99-87-6, p-Cymene 99-93-4,
4-Hydroxyacetophenone 100-51-6, Benzyl alcohol, biological studies
100-52-7, Benzaldehyde, biological studies 103-44-6, 2-Ethylhexylvinyl 103-45-7 104-46-1, Anethol 104-76-7, 2-Ethyl-1-hexanol 104-87-0, 4-Methylbenzaldehyde 106-24-1, Geraniol 108-39-4, biological studies 108-95-2, Phenol, biological studies 109-52-4, Pentanoic acid, biological studies 110-15-6, Butanedioic acid, biological studies 110-93-0 111-14-8, Heptanoic acid 111-27-3, 1-Hexanol, biological 111-70-6, 1-Heptanol 111-71-7, Heptanal 111-87-5, 1-Octanol, studies biological studies 112-05-0, Nonanoic acid 112-12-9, 2-Undecanone 112-31-2, Decanal 112-39-0, Methyl hexadecanoate 112-53-8, 1-Dodecanol 112-72-1, 1-Tetradecanol 115-18-4, 2-Methyl-3-buten-2-ol 115-95-7, Linalyl acetate 119-84-6, 3,4-Dihydrocoumarin 122-00-9 123-11-5, 4-Methoxybenzaldehyde, biological studies 123-35-3, β -Myrcene 123-51-3, 3-Methyl-1-butanol 124-07-2, Octanoic acid, biological studies 124-19-6, Nonanal 124-25-4, Tetradecanal 124-76-5, 124-13-0, Octanal Isoborneol 125-12-2, Isobornyl acetate 127-41-3, α -Ionone 127-91-3, β -Pinene 134-28-1 135-02-4, 140-11-4, Benzyl acetate 141-93-5, 2-Methoxybenzaldehyde 1,3-Diethylbenzene 142-62-1, Hexanoic acid, biological studies 143-07-7, Dodecanoic acid, biological studies 143-08-8, 1-Nonanol 288-13-1, 1H-Pyrazole 334-48-5, Decanoic acid 470-82-6, 1,8-Cineol 471-15-8, β -Thujone 473-06-3, Chrysanthenone 475-03-6, 1,1,6-Trimethyl-1,2,3,4-tetrahydronaphthalene 491-07-6, Isomenthone 497-03-0 499-75-2, Carvacrol 502-69-2, 6,10,14-Trimethyl-2-pentadecanone 505-48-6, Suberic acid 507-70-0, Borneol 515-00-4, Myrtenol 536-60-7, 4-Isopropylbenzyl alcohol 544-63-8, Tetradecanoic acid, biological studies 546-80-5, α -Thujone 564-94-3, Myrtenal 577-16-2 584-02-1, 3-Pentanol 584-03-2, 1,2-Butanediol 585-74-0 586-62-9, Terpinolene 586-82-3 590-67-0, 1-Methylcyclohexanol 611-14-3, 1-Methyl-2-ethylbenzene 620-14-4, 1-Methyl-3-ethylbenzene 628-46-6, 5-Methylhexanoic acid 628-97-7, Ethyl hexadecanoate 628-99-9, 2-Nonanol 629-11-8, 1,6-Hexanediol 629-80-1, Hexadecanal 629-96-9, 1-Eicosanol 629-99-2, Pentacosane 638-53-9, Tridecanoic acid 693-54-9, 2-Decanone 698-76-0, δ -Octalactone 705-86-2, δ -Decalactone 821-55-6, 874-63-5 928-94-9, (Z)-2-Hexen-1-ol 928-95-0, 2-Nonanone (E)-2-Hexen-1-ol 928-96-1, (Z)-3-Hexen-1-ol 928-97-2, (E)-3-Hexen-1-ol1002-84-2, Pentadecanoic acid 1070-35-5, Allyl 4-oxopentanoate 1139-30-6, Caryophyllene oxide 1490-04-6, Menthol 1569-50-2,

```
3-Penten-2-ol 1576-95-0, (Z)-2-Penten-1-ol 1576-96-1,
     (E)-2-Penten-1-ol 1604-34-8, 6,10-Dimethylundecan-2-one
                                                                     1653-30-1,
     2-Undecanol 1669-44-9, 3-Octen-2-one 1678-93-9, Butylcyclohexane
     1862-61-9 2111-75-3, Perillaaldehyde 2345-27-9, 2-Tetradecanone 2345-28-0, 2-Pentadecanone 2408-37-9, 2,2,6-Trimethylcyclohexanone
     2548-87-0, (E)-2-Octenal 2628-17-3 2867-05-2, \alpha-Thujene
     2922-51-2, 2-Heptadecanone 3419-02-1 3623-51-6, Neomenthol
     3724-65-0, 2-Butenoic acid 3765-28-4 3796-70-1, Geranylacetone
     3856-25-5, \alpha-Copaene 4173-41-5 4313-02-4, (E,Z)-2,4-Heptadienal
     4313-03-5, (E,E)-2,4-Heptadienal 4602-84-0, Farnesol 4630-07-3,
     Valencene 5273-86-9, \beta-Asarone 5910-87-2, (E,E)-2,4-Nonadienal
     5989-33-3
                6032-29-7, 2-Pentanol 6175-49-1, 2-Dodecanone
     (Z)-4-Hepten-1-ol 6248-88-0, Fenchane 6728-26-3, (E)-2-Hexenal
     6728-31-0, (Z)-4-Heptenal 6971-51-3, 3-Methoxybenzyl alcohol
     7045-71-8, 2-Methylundecane 7149-65-7, Ethyl pyroglutamate 7212-44-4,
     Nerolidol 7299-42-5, \delta-Terpineol 7373-13-9, 2-Octadecanone
     10031-82-0, 4-Ethoxybenzaldehyde 10547-84-9 13466-78-9,
     \Delta 3-Carene 13678-74-5 14009-71-3, (Z)-Linalool oxide pyranoid
     14398-35-7, 3,4-Didehydro-\beta-ionone 14575-93-0 16303-61-0,
     2-(5-Methyl-2-furanyl)furan 17092-92-1, Dihydroactinidiolide
     17699-16-\overline{0} 18787-\overline{63}-8, 2-Hexadecanone 18829-55-5, (E)-2-Heptenal
     18829-56-6, (E)-2-Nonenal 19435-97-3, \delta-Cadinol 20019-64-1
     20053-88-7, Hotrienol 20279-49-6, Pentyl 4-oxo-pentanoate
                                                                        20407-84-5,
     (E)-2-Dodecenal 22122-36-7, 3-Methyl-2(5H)-furanone 23267-57-4,
     5,6-\text{Epoxy}-\beta-\text{ionone} 23313-79-3 23986-74-5, Germacrene D 25152-84-5, (E,E)-2,4-Decadienal 28069-72-9 29606-79-9, Isopulegone
     30086-02-3, (E,E)-3,5-Octadien-2-one 30361-28-5, (E,E)-2,4-Oct 30364-38-6, 1,1,6-Trimethyl-1,2-dihydronaphthalene 31499-72-6,
                                              30361-28-5, (E,E)-2,4-Octadienal
     Dihydro-\alpha-ionone 33081-34-4, Lilac alcohol, a 33081-35-5, Lilac
     alcohol, b 33393-93-0 34995-77-2 36653-82-4, 1-Hexadecanol
                                                                 54814-64-1
     38736-62-8
                   39028-58-5
                                53448-07-0, (E)-2-Undecenal
                  58985-18-5, Dihydroterpinyl acetate 64142-78-5,
     55194-06-4
     8-Hydroxylinalool 68922-10-1 72747-25-2, Aromadendrene
                                                                      97844-14-9
     137222-06-1 139064-04-3
                                  139113-27-2 139123-06-1 139123-07-2
     RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
     BIOL (Biological study); OCCU (Occurrence)
        (of woodruff aroma)
                                 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
OS.CITING REF COUNT:
                                 (3 CITINGS)
     Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung (1991),
     193(4), 317-20
     CODEN: ZLUFAR; ISSN: 0044-3026
     woodruff flavor volatile
     Flavor
         (woodruff, composition of)
     57-10-3, Hexadecanoic acid, biological studies 57-11-4, Octadecanoic
     acid, biological studies 60-12-8, 2-Phenylethanol 64-19-7, Acetic
     acid, biological studies 65-85-0, Benzoic acid, biological studies
     66-25-1, Hexanal 71-36-3, 1-Butanol, biological studies 71-41-0,
     1-Pentanol, biological studies 76-22-2 76-49-3, Bornyl acetate
               78-70-6, Linalool 78-83-1, 2-Methyl-1-propanol, biological 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological studies
     78-36-4
     studies
     79-77-6, β-Ionone 79-92-5, Camphene 89-80-5, Menthone 89-81-6, Piperitone 89-82-7, Pulegone 89-83-8, Thymol 90-00-6, 2-Ethylphenol
     Piperitone 89-82-7, Pulegone 89-83-8, Thymol
     91-64-5, Coumarin 93-15-2, Eugenylmethyl ether
                                                            93-55-0,
     1-Phenylpropan-1-one 95-48-7, biological studies 98-55-5, \alpha-Terpineol 99-49-0, Carvone 99-50-3, 3,4-Dihydroxybenzoic acid
     99-85-4, γ-Terpinen 99-87-6, p-Cymene 99-93-4,
     4-Hydroxyacetophenone 100-51-6, Benzyl alcohol, biological studies
     100-52-7, Benzaldehyde, biological studies 103-44-6, 2-Ethylhexylvinyl
     ether 103-45-7 104-46-1, Anethol 104-76-7, 2-Ethyl-1-hexanol
```

SO

ST

ΙT

ΙT

```
104-87-0, 4-Methylbenzaldehyde 106-24-1, Geraniol 108-39-4, biological
studies 108-95-2, Phenol, biological studies 109-52-4, Pentanoic acid,
biological studies 110-15-6, Butanedioic acid, biological studies
110-93-0 111-14-8, Heptanoic acid 111-27-3, 1-Hexanol, biological
studies 111-70-6, 1-Heptanol 111-71-7, Heptanal 111-87-5, 1-Octanol,
biological studies 112-05-0, Nonanoic acid 112-12-9, 2-Undecanone
112-31-2, Decanal 112-39-0, Methyl hexadecanoate 112-53-8, 1-Dodecanol
112-72-1, 1-Tetradecanol 115-18-4, 2-Methyl-3-buten-2-ol
                                                            115-95-7,
Linalyl acetate 119-84-6, 3,4-Dihydrocoumarin 122-00-9
4-Methoxybenzaldehyde, biological studies 123-35-3, \beta-Myrcene
123-51-3, 3-Methyl-1-butanol 124-07-2, Octanoic acid, biological studies
124-13-0, Octanal 124-19-6, Nonanal 124-25-4, Tetradecanal
Isoborneol 125-12-2, Isobornyl acetate 127-41-3, \alpha-Ionone
127-91-3, \beta-Pinene 134-28-1 135-02-4,
2-Methoxybenzaldehyde 140-11-4, Benzyl acetate 141-93-5,
1,3-Diethylbenzene 142-62-1, Hexanoic acid, biological studies
143-07-7, Dodecanoic acid, biological studies 143-08-8, 1-Nonanol
288-13-1, 1H-Pyrazole 334-48-5, Decanoic acid 470-82-6, 1,8-Cineol
471-15-8, \beta-Thujone 473-06-3, Chrysanthenone 475-03-6,
1,1,6-Trimethyl-1,2,3,4-tetrahydronaphthalene 491-07-6, Isomenthone
497-03-0 499-75-2, Carvacrol 502-69-2,
6,10,14-Trimethyl-2-pentadecanone 505-48-6, Suberic acid 507-70-0,
Borneol 515-00-4, Myrtenol 536-60-7, 4-Isopropylbenzyl alcohol
544-63-8, Tetradecanoic acid, biological studies 546-80-5,
\alpha-Thujone 564-94-3, Myrtenal 577-16-2 584-02-1, 3-Pentanol
584-03-2, 1,2-Butanediol 585-74-0 586-62-9, Terpinolene 586-82-3
590-67-0, 1-Methylcyclohexanol 611-14-3, 1-Methyl-2-ethylbenzene
619-62-5 620-14-4, 1-Methyl-3-ethylbenzene 628-46-6, 5-Methylhexanoic
acid 628-97-7, Ethyl hexadecanoate 628-99-9, 2-Nonanol 629-11-8,
1,6-Hexanediol 629-80-1, Hexadecanal 629-96-9, 1-Eicosanol 629-99-2,
Pentacosane 638-53-9, Tridecanoic acid 693-54-9, 2-Decanone 693-80-1
698-76-0, \delta-Octalactone 705-86-2, \delta-Decalactone 821-55-6,
2-Nonanone 874-63-5 928-94-9, (Z)-2-Hexen-1-ol 928-95-0,
(E)-2-\text{Hexen}-1-\text{ol} 928-96-1, (Z)-3-\text{Hexen}-1-\text{ol} 928-97-2, (E)-3-\text{Hexen}-1-\text{ol}
1002-84-2, Pentadecanoic acid 1070-35-5, Allyl 4-oxopentanoate
1139-30-6, Caryophyllene oxide 1490-04-6, Menthol 1569-50-2,
3-Penten-2-ol 1576-95-0, (Z)-2-Penten-1-ol
                                              1576-96-1,
(E)-2-Penten-1-ol 1604-34-8, 6,10-Dimethylundecan-2-one
2-Undecanol 1669-44-9, 3-Octen-2-one 1678-93-9, Butylcyclohexane
1862-61-9
          2111-75-3, Perillaaldehyde 2345-27-9, 2-Tetradecanone
                             2408-37-9, 2,2,6-Trimethylcyclohexanone
2345-28-0, 2-Pentadecanone
2548-87-0, (E)-2-Octenal 2628-17-3 2867-05-2, \alpha-Thujene
2922-51-2, 2-Heptadecanone
                            3419-02-1 3623-51-6, Neomenthol
3724-65-0, 2-Butenoic acid
                           3765-28-4 3796-70-1, Geranylacetone
3856-25-5, \alpha-Copaene 4173-41-5 4313-02-4, (E,Z)-2, 4-Heptadienal
                                   4602-84-0, Farnesol 4630-07-3,
4313-03-5, (E,E)-2,4-Heptadienal
                                   5910-87-2, (E,E)-2,4-Nonadienal
Valencene
           5273-86-9, \beta-Asarone
           6032-29-7, 2-Pentanol 6175-49-1, 2-Dodecanone 6191-71-5,
5989-33-3
(2)-4-Hepten-1-ol 6248-88-0, Fenchane 6728-26-3, (E)-2-Hexenal
6728-31-0, (Z)-4-Heptenal 6971-51-3, 3-Methoxybenzyl alcohol
7045-71-8, 2-Methylundecane 7149-65-7, Ethyl pyroglutamate
                                                              7212-44-4,
Nerolidol 7299-42-5, \delta-Terpineol 7373-13-9, 2-Octadecanone
10031-82-0, 4-Ethoxybenzaldehyde 10547-84-9 13466-78-9,
\Delta 3-Carene 13678-74-5 14009-71-3, (Z)-Linalool oxide pyranoid 14398-35-7, 3,4-Didehydro-\beta-ionone 14575-93-0 16303-61-0,
2-(5-Methyl-2-furanyl)furan 17092-92-1, Dihydroactinidiolide
17699-16-0 18787-63-8, 2-Hexadecanone 18829-55-5, (E)-2-Heptenal 18829-56-6, (E)-2-Nonenal 19435-97-3, \delta-Cadinol 20019-64-1
20053-88-7, Hotrienol 20279-49-6, Pentyl 4-oxo-pentanoate 20407-84-5,
(E)-2-Dodecenal 22122-36-7, 3-Methyl-2(5H)-furanone 23267-57-4,
5,6-\text{Epoxy}-\beta-\text{ionone} 23313-79-3 23986-74-5, Germacrene D
```

25152-84-5, (E,E)-2,4-Decadienal 28069-72-9 29606-79-9, Isopulegone 30086-02-3, (E,E)-3,5-Octadien-2-one 30361-28-5, (E,E)-2,4-Octadienal 30364-38-6, 1,1,6-Trimethyl-1,2-dihydronaphthalene 31499-72-6, 33081-34-4, Lilac alcohol, a 33081-35-5, Lilac Dihydro- α -ionone alcohol, b 33393-93-0 34995-77-2 36653-82-4, 1-Hexadecanol 38736-62-8 39028-58-5 53448-07-0, (E)-2-Undecenal 54814-64-1 55194-06-4 58985-18-5, Dihydroterpinyl acetate 64142-78-5, 8-Hydroxylinalool 68922-10-1 72747-25-2, Aromadendrene 137222-06-1 139064-04-3 139113-27-2 139123-06-1 139123-07-2 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (of woodruff aroma)

L29 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1990:610224 HCAPLUS

DOCUMENT NUMBER: 113:210224

ORIGINAL REFERENCE NO.: 113:35524h,35525a

TITLE: Characterization of ham flavor using an atomic

emission detector

AUTHOR(S): Baloga, David W.; Reineccius, Gary A.; Miller, Joel W. CORPORATE SOURCE: Dep. Food Sci. Nutr., Univ. Minnesota, St. Paul, MN,

55108, USA

SOURCE: Journal of Agricultural and Food Chemistry (1990),

38(11), 2021-6

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal LANGUAGE: English

ABSTRACT:

Volatile favor compds. were isolated from a cured, precooked premium ham by using a Likens-Nickerson apparatus Four individual 250-g ham samples were used to provide flavor isolates, which were pooled and concentrated for extensive gas chromatog. anal. Atomic emission, flame ionization, flame photometry, N-P, and mass spectrometry were used to qual. determine specific constituents of the pooled solvent fraction. At emission were useful in the selective detection of N-, O-, and S-containing compds. More than 60 compds. were tentatively identified, including phenols, aliphatic alcs., ketones, and aldehydes, and cyclooctasulfur.

- TI Characterization of ham flavor using an atomic emission detector
- SO Journal of Agricultural and Food Chemistry (1990), 38(11), 2021-6 CODEN: JAFCAU; ISSN: 0021-8561
- AB . . . from a cured, precooked premium ham by using a Likens-Nickerson apparatus Four individual 250-g ham samples were used to provide flavor isolates, which were pooled and concentrated for extensive gas chromatog. anal. Atomic emission, flame ionization, flame photometry, N-P, and mass. . .
- ST ham flavor analysis; gas chromatog flavor; atomic emission spectrometry flavor
- IT Flavor
 - Odor and Odorous substances

(determination of, of ham by gas chromatog. with atomic emission detection) 66-25-1, Hexanal 78-93-3, 2-Butanone, analysis 84-74-2 90-00-6, ΙT 2-Ethylphenol 90-05-1 93-51-6, 4-Methylquaiacol 95-48-7, analysis 95-65-8 95-87-4 97-53-0, 4-Allylquaiacol 98-01-1, 2-Furancarboxaldehyde, analysis 98-86-2, analysis 100-52-7, Benzaldehyde, analysis 105-87-3, Geranyl acetate 106-24-1 106-44-5, 108-39-4, analysis 108-95-2, Phenol, analysis analysis 112-54-9, Dodecanal 121-98-2 122-78-1, Methylpyrazine Benzeneacetaldehyde 124-25-4, Tetradecanal 128-37-0, analysis 135-02-4, 2-Methoxybenzaldehyde 141-78-6, Acetic acid ethyl ester, analysis $\overline{150-78-7}$ $\overline{526-75-0}$, 2,3-Dimethylphenol 556-82-1, 3-Methyl-2-buten-1-ol 560-21-4, 2,3,3-Trimethylpentane 576-26-1 590-86-3 600-14-6, 2,3-Pentanedione 625-74-1, 2-Methyl-1-nitropropane

```
629-80-1, Hexadecanal 638-66-4, Octadecanal 642-71-7,
    3,4,5-Trimethoxyphenol 1192-62-7, 2-Acetylfuran 1453-24-3,
    1-Ethylcyclohexene 1577-52-2, 9,12-Octadecadien-1-ol 1639-04-9,
    2-Methyl-3-pentanethiol 2345-28-0, 2-Pentadecanone 2758-18-1
    2765-11-9, Pentadecanal 2785-89-9, 4-Ethylguaiacol 3581-87-1,
                      3658-80-8, Dimethyl trisulfide
                                                      3877-15-4,
    2-Methylthiazole
    1-Methylthiopropane
                          5090-41-5, 9-Octadecenal 5756-24-1, Dimethyl
    tetrasulfide 5912-86-7, cis-Isoeugenol 7786-61-0, 4-Vinylquaiacol
    10544-50-0, Cyclooctasulfur, analysis 12767-10-1, Octadecadienol
    26537-70-2, 9,12-Octadecadienal 34314-83-5, 4-Methyl-2,3-dihydrofuran
    55683-21-1 56554-96-2, 2-Octadecenal 58539-27-8 129216-51-9
    129216-52-0, 9,17-Octadecadien-1-ol
    RL: ANT (Analyte); ANST (Analytical study)
        (determination of, of ham aroma by gas chromatog. with atomic emission
       detector)
                              THERE ARE 12 CAPLUS RECORDS THAT CITE THIS
OS.CITING REF COUNT:
                        12
                              RECORD (12 CITINGS)
    Characterization of ham flavor using an atomic emission detector
ΤI
SO
    Journal of Agricultural and Food Chemistry (1990), 38(11), 2021-6
    CODEN: JAFCAU; ISSN: 0021-8561
AΒ
    Volatile favor compds. were isolated from a cured, precooked premium ham
    by using a Likens-Nickerson apparatus Four individual 250-g ham samples were
    used to provide flavor isolates, which were pooled and concentrated for
    extensive gas chromatog. anal. Atomic emission, flame ionization, flame
    photometry, N-P, and mass spectrometry were used to qual. determine specific
    constituents of the pooled solvent fraction. At emission were useful in
    the selective detection of N-, O-, and S-containing compds. More than 60
    compds. were tentatively identified, including phenols, aliphatic alcs.,
    ketones, and aldehydes, and cyclooctasulfur.
ST
    ham flavor analysis; gas chromatog flavor; atomic emission
    spectrometry flavor
    Flavor
ΙT
    Odor and Odorous substances
        (determination of, of ham by gas chromatog. with atomic emission detection)
    66-25-1, Hexanal 78-93-3, 2-Butanone, analysis 84-74-2 90-00-6,
ΙT
    2-Ethylphenol
                   90-05-1 93-51-6, 4-Methylguaiacol
                                                         95-48-7, analysis
    95-65-8
                        97-53-0, 4-Allylguaiacol
              95-87-4
                                                  98-01-1,
    2-Furancarboxaldehyde, analysis 98-86-2, analysis 100-52-7,
    Benzaldehyde, analysis
                            105-87-3, Geranyl acetate
                                                       106-24-1
                                                                    106-44-5,
    analysis 108-39-4, analysis 108-95-2, Phenol, analysis
    Methylpyrazine
                    112-54-9, Dodecanal
                                          121-98-2
                                                     122-78-1,
    Benzeneacetaldehyde 124-25-4, Tetradecanal
                                                  128-37-0, analysis
    135-02-4, 2-Methoxybenzaldehyde 141-78-6, Acetic acid ethyl
    ester, analysis 150-78-7 526-75-0, 2,3-Dimethylphenol
                                                               556-82-1,
    3-Methyl-2-buten-1-ol 560-21-4, 2,3,3-Trimethylpentane
                                                               576-26-1
    590-86-3 600-14-6, 2,3-Pentanedione 625-74-1, 2-Methyl-1-nitropropane
    629-80-1, Hexadecanal 638-66-4, Octadecanal 642-71-7,
    3,4,5-Trimethoxyphenol 1192-62-7, 2-Acetylfuran 1453-24-3,
    1-Ethylcyclohexene 1577-52-2, 9,12-Octadecadien-1-ol 1639-04-9,
    2-Methyl-3-pentanethiol 2345-28-0, 2-Pentadecanone 2758-18-1 2765-11-9, Pentadecanal 2785-89-9, 4-Ethylguaiacol 3581-87-1,
                                                           3581-87-1,
    2-Methylthiazole 3658-80-8, Dimethyl trisulfide 3877-15-4,
    1-Methylthiopropane 5090-41-5, 9-Octadecenal 5756-24-1, Dimethyl
    tetrasulfide 5912-86-7, cis-Isoeugenol 7786-61-0, 4-Vinylguaiacol
    10544-50-0, Cyclooctasulfur, analysis 12767-10-1, Octadecadienol
    26537-70-2, 9,12-Octadecadienal 34314-83-5, 4-Methyl-2,3-dihydrofuran
    55683-21-1
                 56554-96-2, 2-Octadecenal 58539-27-8 129216-51-9
    129216-52-0, 9,17-Octadecadien-1-ol
    RL: ANT (Analyte); ANST (Analytical study)
        (determination of, of ham aroma by gas chromatog. with atomic emission
```

detector)

L29 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN 1989:630914 HCAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 111:230914 ORIGINAL REFERENCE NO.: 111:38361a,38364a Styrene production by Penicillium camemberti Thom TITLE: AUTHOR(S): Adda, J.; Dekimpe, J.; Vassal, L.; Spinnler, H. E. CORPORATE SOURCE: Lab. Rech. Aromes, INRA, Dijon, Fr. SOURCE: Lait (1989), 69(2), 115-20 CODEN: LAITAG; ISSN: 0023-7302 DOCUMENT TYPE: Journal French LANGUAGE: **ABSTRACT:** The celluloid taste observed in some mold-ripened cheeses is related to the presence of styrene in these cheeses. The accumulation of this mol. was only detected on cultures of some strains of Penicillium camemberti. It seems to be related to a change in oxidative metabolism in these strains. Volatile products of soft mold-ripened cheeses were examined by capillary gas chromatog. SO Lait (1989), 69(2), 115-20 CODEN: LAITAG; ISSN: 0023-7302 ST Penicillium styrene cheese flavor; soft cheese flavor styrene ΙΤ Penicillium camembertii (styrene formation by, cheese off-flavor in relation to) ΙT Flavor (off-, of mold-ripened soft cheese, styrene formation by Penicillium camemberti in relation to) ΙT Cheese (soft, flavor of mold-ripened, Penicillium camemberti styrene formation) 54-11-5, Nicotine 60-12-8, Phenyl-2-ethanol 67-71-0, Dimethyl sulfone ΤТ 71-41-0, Pentanol, biological studies 87-44-5 91-20-3, Naphthalene, biological studies 96-17-3, Methyl-2-butanal 98-55-5, α -Terpineol 100-52-7, Benzaldehyde, biological studies 100-66-3, Methoxybenzene, biological studies 105-54-4, Ethyl butyrate 106-32-1 106-68-3, 3-Octanone 107-87-9, 2-Pentanone 108-88-3, Toluene, 110-38-3, Ethyl decanoate biological studies 110-43-0, Heptan-2-one 111-13-7, Octan-2-one 111-27-3, Hexanol, biological studies 111-87-5, Octan-1-ol, biological studies 112-12-9, Undecan-2-one 112-30-1, Decan-1-ol 112-53-8, Dodecanol 120-72-9, 1H-Indole, biological studies 123-51-3, Methyl-3-butan-1-ol 128-37-0, BHT, 124-19-6, Nonanal biological studies 140-29-4, Benzylcyanide 151-10-0, 1,3-Dimethoxybenzene 589-98-0, Octan-3-ol 591-78-6, Hexan-2-one 593-08-8, Tridecan-2-one 624-92-0, Dimethyldisulfide 628-99-9, Nonan-2-ol 693-54-9, Decan-2-one 821-55-6, Nonan-2-one 1330-20-7. Xylene, biological studies 1484-17-9, Ethyl S-thiobenzoate 1653-30-1, 3391-86-4, Oct-1-en-3-ol 6032-29-7, Pentan-2-ol Undecan-2-ol 7380-48-5, Oct-3-enyl acetate 20013-10-9, Non-8-en-3-one 25321-22-6, Dichlorobenzene 25550-14-5, Ethyl methyl benzene 27323-28-0, Methyl 27936-14-7, Undecen-2-one 57782-14-6, Tridecenone 69093-74-9, indole Dec-3-en-1-ol 83861-74-9, Octa-1,5-dien-3-ol RL: BIOL (Biological study) (of mold-ripened soft cheese aroma) 100-42-5, biological studies RL: BIOL (Biological study) (of mold-ripened soft cheese off-flavor, Penicillium camemberti formation of) OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS) SO Lait (1989), 69(2), 115-20

CODEN: LAITAG; ISSN: 0023-7302

```
Penicillium styrene cheese flavor; soft cheese flavor styrene
ST
ΙT
    Penicillium camembertii
        (styrene formation by, cheese off-flavor in relation to)
    Flavor
IΤ
        (off-, of mold-ripened soft cheese, styrene formation by Penicillium
        camemberti in relation to)
ΙT
    Cheese
        (soft, flavor of mold-ripened, Penicillium camemberti styrene
        formation)
    54-11-5, Nicotine
                       60-12-8, Phenyl-2-ethanol
                                                    67-71-0, Dimethyl sulfone
ΙT
    71-41-0, Pentanol, biological studies 87-44-5
                                                     91-20-3, Naphthalene,
    biological studies 96-17-3, Methyl-2-butanal
                                                     98-55-5,
    \alpha-Terpineol 100-52-7, Benzaldehyde, biological studies
                                                               100-66-3,
    Methoxybenzene, biological studies 105-54-4, Ethyl butyrate
    106-68-3, 3-Octanone 107-87-9, 2-Pentanone 108-88-3, Toluene,
    biological studies 110-38-3, Ethyl decanoate 110-43-0, Heptan-2-one
    111-13-7, Octan-2-one 111-27-3, Hexanol, biological studies 111-87-5,
    Octan-1-ol, biological studies 112-12-9, Undecan-2-one 112-30-1,
    Decan-1-ol 112-53-8, Dodecanol 120-72-9, 1H-Indole, biological studies
    123-51-3, Methyl-3-butan-1-ol 124-19-6, Nonanal
                                                      128-37-0, BHT,
    biological studies 140-29-4, Benzylcyanide 151-10-0,
    1,3-Dimethoxybenzene 589-98-0, Octan-3-ol
                                                  591-78-6, Hexan-2-one
    593-08-8, Tridecan-2-one 624-92-0, Dimethyldisulfide 628-99-9,
    Nonan-2-ol 693-54-9, Decan-2-one 821-55-6, Nonan-2-one
                                                               1330-20-7,
    Xylene, biological studies 1484-17-9, Ethyl S-thiobenzoate
    Undecan-2-ol 3391-86-4, Oct-1-en-3-ol 6032-29-7, Pentan-2-ol
    7380-48-5, Oct-3-enyl acetate 20013-10-9, Non-8-en-3-one
                                                               25321-22-6,
    Dichlorobenzene 25550-14-5, Ethyl methyl benzene 27323-28-0, Methyl
             27936-14-7, Undecen-2-one 57782-14-6, Tridecenone 69093-74-9,
    indole
    Dec-3-en-1-ol
                   83861-74-9, Octa-1,5-dien-3-ol
    RL: BIOL (Biological study)
        (of mold-ripened soft cheese aroma)
    100-42-5, biological studies
ΤТ
    RL: BIOL (Biological study)
        (of mold-ripened soft cheese off-flavor, Penicillium
        camemberti formation of)
L29 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER:
                        1988:20686 HCAPLUS
DOCUMENT NUMBER:
                        108:20686
ORIGINAL REFERENCE NO.: 108:3501a,3504a
TITLE:
                        The metabolic disposition of [methoxy-14C]-labeled
                        trans-anethole, estragole and p-propylanisole in human
                        volunteers
                        Sangster, Susan A.; Caldwell, John; Hutt, Andrew J.;
AUTHOR(S):
                        Anthony, Andrew; Smith, Robert L.
                        Med. Sch., St. Mary's Hosp., London, W2 1PG, UK
CORPORATE SOURCE:
                        Xenobiotica (1987), 17(10), 1223-32
SOURCE:
                        CODEN: XENOBH; ISSN: 0049-8254
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                        English
ABSTRACT:
The metabolic fates of the naturally occurring food flavors trans-anethole
and estragole, and their synthetic congener p-propylanisole, were investigated
in human volunteers by using the [methoxy-14C]-labeled compds. The doses used
were close to those encountered in the diet, 1 mg, 100 \mu g, and 100 \mu g
resp. In each case, the major routes of elimination of 14C were in the urine
and in the expired air as 14CO2. Urinary metabolites were separated by solvent
extraction, TLC and HPLC, and characterized by comparison of chromatog. mobilities
with stds. and by radioisotope dilution Nine 14C urinary metabolites were found
```

after trans-anethole administration, 4 after p-propylanisole, and 5 after

estragole. All were products of side-chain oxidns. The principal metabolites of p-propylanisole were 4-methoxyhippuric acid (12%) and 1-(4'-methoxyphenyl) propan-1-ol (2%) and -2-ol (8%). The major metabolite of trans-anethole was 4-methoxyhippuric acid (56% of dose), accompanied by much smaller amts. of the 2 isomers of 1-(4'-methoxyphenyl) propane-1,2-diol (together 3%). After estragole administration, the 2 volunteers eliminated 0.2 and 0.4% of the dose, resp., as 1'-hydroxyestragole. The human metabolic data is discussed with reference to the comparative metabolic disposition of these compds. in the mouse and rat, species commonly used for safety assessment.

- SO Xenobiotica (1987), 17(10), 1223-32 CODEN: XENOBH; ISSN: 0049-8254
- AB The metabolic fates of the naturally occurring food flavors trans-anethole and estragole, and their synthetic congener p-propylanisole, were investigated in human volunteers by using the [methoxy-14C]-labeled compds. The doses. . .
- IT Flavor

(anethole and estragole of, metabolism of, in humans)

IT Flavoring materials

(propylanisol of, metabolism of, in humans)

IT 104-45-0, p-Propylanisole 140-67-0, Estragole 4180-23-8, trans-Anethole

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(metabolism of, in humans, food flavor use in relation to)

IT 5349-60-0

RL: BIOL (Biological study)

(propylanisole flavoring metabolite, in humans)

- OS.CITING REF COUNT: 34 THERE ARE 34 CAPLUS RECORDS THAT CITE THIS RECORD (34 CITINGS)
- SO Xenobiotica (1987), 17(10), 1223-32 CODEN: XENOBH; ISSN: 0049-8254
- AB The metabolic fates of the naturally occurring food flavors trans-anethole and estragole, and their synthetic congener p-propylanisole, were investigated in human volunteers by using the [methoxy-14C]-labeled compds. The doses used were close to those encountered in the diet, 1 mg, 100 μ g, and 100 μ g resp. In each case, the major routes of elimination of 14C were in the urine and in the expired air as 14CO2. Urinary metabolites were separated by solvent extraction,

TLC and HPLC, and characterized by comparison of chromatog. mobilities with stds. and by radioisotope dilution Nine 14C urinary metabolites were found after trans-anethole administration, 4 after p-propylanisole, and 5 after estragole. All were products of side-chain oxidns. The principal metabolites of p-propylanisole were 4-methoxyhippuric acid (12%) and 1-(4'-methoxyphenyl)propan-1-ol (2%) and -2-ol (8%). The major metabolite of trans-anethole was 4-methoxyhippuric acid (56% of dose), accompanied by much smaller amts. of the 2 isomers of

1-(4'-methoxyphenyl) propane-1,2-diol (together 3%). After estragole administration, the 2 volunteers eliminated 0.2 and 0.4% of the dose, resp., as 1'-hydroxyestragole. The human metabolic data is discussed with reference to the comparative metabolic disposition of these compds. in the mouse and rat, species commonly used for safety assessment.

IT Flavor

(anethole and estragole of, metabolism of, in humans)

IT Flavoring materials

(propylanisol of, metabolism of, in humans)

IT 104-45-0, p-Propylanisole 140-67-0, Estragole 4180-23-8, trans-Anethole

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(metabolism of, in humans, food flavor use in relation to) ΤT 5349-60-0 RL: BIOL (Biological study) (propylanisole flavoring metabolite, in humans) ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN L29 ACCESSION NUMBER: 1985:130580 HCAPLUS DOCUMENT NUMBER: 102:130580 ORIGINAL REFERENCE NO.: 102:20477a,20480a Consumption ratio and food predominance of flavoring TITLE: materials - second cumulative series AUTHOR(S): Stofberg, Jan; Grundschober, Friedrich CORPORATE SOURCE: PFW, Div., Hercules Inc., Middletown, NY, 10940, USA SOURCE: Perfumer & Flavorist (1984), 9(4), 53-6, 58-9, 62, 65-72, 76-83 CODEN: PEFLDI; ISSN: 0361-8587 DOCUMENT TYPE: Journal LANGUAGE: English ABSTRACT: Detailed data are tabulated on the consumption ratio of food flavoring materials, i.e., the ratio between the quantity of a flavoring material consumed as an ingredient of food and the quantity of the same flavorant consumed as a component of added flavoring material. The food consumption ratio was calculated from the USA literature data published after 1983. Of 347 flavoring materials covered, 296 were found as food predominant or those having the consumption ratio of >1; 205 of them had a consumption ratio of >10. TΙ Consumption ratio and food predominance of flavoring materials - second cumulative series Perfumer & Flavorist (SO 1984), 9(4), 53-6, 58-9, 62, 65-72, 76-83 CODEN: PEFLDI; ISSN: 0361-8587 Detailed data are tabulated on the consumption ratio of food flavoring AΒ materials, i.e., the ratio between the quantity of a flavoring material consumed as an ingredient of food and the quantity of the same flavorant consumed as a component of added flavoring material. The food consumption ratio was calculated from the USA literature data published after 1983. Of 347 flavoring materials covered, 296 were found as food predominant or those having the consumption ratio of >1; 205 of them had. ST flavoring material food diet ΙT Flavoring materials (food consumption ratio of) ΙT 57-06-7 57-10-3, biological studies 57-11-4, biological studies 60-12-8 60-33-3, biological studies 64-18-6, biological studies 67-63-0, biological studies 67-64-1, biological studies 66-25-1 71-36-3, biological studies 71-23-8, biological studies biological studies 74-93-1, biological studies 75-07-0, biological 76-49-3 78-70-6 78-83-1, biological studies 75-18-3 studies 78-84-2 78-92-2 78-93-3, biological studies 78-98-8 79-09-4, biological studies 79-20-9 79-31-2 79-76-5 79-77-6 79-92-5 87-44-5 90-02-8, biological studies 80-56-8 80-71-7 83-34-1 90-05-1 90-12-0 92-52-4, biological studies 93-15-2 93-16-3 93-51-6 93-58-3 93-89-0 94-46-2 95-48-7, biological studies 95-65-8 95-87-4 96-17-3 96-48-0 97-54-1 97-62-1 97-87-0 98-01-1, biological studies 98-02-2 98-85-1 98-00-0 98-55-5 98-86-2, biological studies 99-83-2 99-85-4 99-86-5 99-87-6 100-42-5, biological studies 100-51-6, biological studies 100-52-7, biological studies 103-36-6 103-45-7 103-95-7 104-09-6 104-50-7 104-57-4 104-61-0 104-67-6 104-76-7 105-21-5 105-37-3 105-54-4 105-68-0 105-79-3 105-87-3 106-18-3 106-21-8 106-22-9 106-23-0

```
106-24-1
               106-25-2 106-27-4 106-29-6 106-30-9
                                                        106-32-1
                                                                    106-33-2
    106-35-4
               106-36-5
                        106-44-5, biological studies 106-70-7
                                                                  107-85-7
    107-87-9
               107-92-6, biological studies 108-10-1
                                                       108-29-2
                                                                  108-39-4.
                                             108-95-2, biological studies
    biological studies
                        108-50-9
                                   108-64-5
    109-08-0
               109-19-3
                         109-21-7
                                   109-52-4, biological studies
                                                                  109-60-4
    109-94-4
               109-97-7
                         110-19-0
                                   110-38-3 110-39-4
                                                         110-43-0
                                                                    110-62-3
                                 110-89-4, biological studies 110-93-0
    110-86-1, biological studies
                                    111-27-3, biological studies
    111-11-5
              111-13-7
                         111-14-8
                                                                  111-70-6
    111-82-0
               111-87-5, biological studies 112-05-0
                                                       112-06-1
                                                                  112-12-9
    112-14-1
              112-17-4
                        112-30-1 112-31-2 112-37-8
                                                         112-54-9
    112-80-1, biological studies 115-95-7 118-71-8
                                                       119-36-8
                                                                  120 - 72 - 9,
    biological studies
                        121-33-5
                                  122-70-3
                                            122-72-5
                                                       122-78-1
    123-19-3
               123-25-1
                         123-32-0
                                   123-35-3
                                              123-38-6, biological studies
               123-66-0 123-72-8
    123-51-3
                                   123-75-1, biological studies
                                                                123-92-2
    123-96-6
              124-06-1 124-07-2, biological studies 124-10-7
                                                                  124-13-0
    124-19-6
              127-41-3 127-91-3
                                   138-87-4
                                              140 - 11 - 4
                                                        140-26-1 140-88-5
    141-12-8
               141-14-0
                        141-16-2
                                   141-78-6, biological studies
                                                                141-97-9
               142-62-1, biological studies
    142-50-7
                                            142-92-7 143-07-7, biological
                         143-13-5
                                   150-84-5
                                              431-03-8
                                                        463-40-1
    studies
              143-08-8
                                                                   464-49-3
    470-82-6
               488-10-8
                         491-04-3
                                    491-09-8
                                              495-62-5
                                                         497-03-0
                                                                    499-75-2
    503-74-2
               505-10-2
                         505-57-7
                                    507-70-0
                                              513-86-0
                                                         540-07-8
                                                                    540-18-1
                                    544-63-8, biological studies
    542-55-2
               543-49-7
                          544-12-7
                                                                546-79-2
    547-63-7
               556-24-1
                          556-82-1
                                    557-48-2
                                               562-74-3
                                                         576-26-1
    582-24-1
               586-62-9
                          589-38-8
                                    589-98-0
                                              590-01-2
                                                         590-86-3
    592-84-7
               593-08-8
                         600-14-6
                                    606-45-1
                                              616-25-1
                                                         620-02-0
                                                                    623-17-6
    623-19-8
               623-36-9
                         623-42-7
                                    623-70-1
                                               624-24-8
                                                         624-92-0
                                                                    626-77-7
    626-82-4
               628-99-9
                         629-19-6
                                    638-11-9
                                               638-25-5
                                                         695-06-7
                                                                    698-76-0
                         710-04-3
    705-86-2
               706-14-9
                                    713-95-1
                                               764-39-6
    RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
       (flavorant, food consumption ratio of)
ΙT
              823-22-3 870-23-5 1072-83-9
                                               1117-52-8 1117-55-1
    821-55-6
    1122-62-9
               1124-11-4
                          1139-30-6
                                      1192-62-7 1193-79-9
                                                              1365-19-1
              1632-73-1
                                       2050-01-3
                                                   2111-75-3
    1438-94-4
                           2035-99-6
                                                              2198-61-0
    2305-05-7
               2305-21-7
                           2345-26-8
                                      2349-07-7
                                                   2363-89-5
                                                              2412-80-8
    2463-53-8
              2463-77-6
                           2497-18-9
                                      2639-63-6
                                                   2721-22-4
                                                              2785-89-9
    3025-30-7
              3142-66-3
                           3188-00-9
                                       3268-49-3
                                                  3301-94-8
                                                              3391-86-4
              3658-80-8
    3658-77-3
                           3777-69-3
                                       3796-70-1
                                                  3848-24-6
                                                              3913-71-1
    4411-89-6
              4437-22-3
                           4630-07-3
                                       4674-50-4
                                                  5392-40-5
                                                              5454-09-1
    5454-28-4
              5457-70-5
                           5905-46-4
                                       5905-47-5
                                                   5910-85-0
                                                              5910-89-4
    5989-27-5
                6028-61-1
                           6032-29-7
                                       6290-37-5
                                                   6309-51-9
                                                              6378-65-0
                                                  7786-44-9
    6380-23-0
                6789-80-6
                           6946-90-3
                                       7452-79-1
                                                              7786-61-0
    10032-15-2
               13162-46-4 13327-56-5 13360-64-0
                                                      13360-65-1
    13532-18-8
                13623-11-5 13679-46-4
                                         13679-85-1
                                                      13925-00-3
    13925-06-9
                13925-07-0 13925-08-1
                                         14667-55-1
                                                      15706-73-7
    15707-23-0
                 16409-46-4 17619-36-2
                                         18640-74-9
                                                      18829-55-5
                            22047-25-2
                                         23328-62-3
    21188-58-9
                 21834-92-4
                                                      23726-93-4
                             29811-50-5
    24295-03-2
                 25152-84-5
                                          31501-11-8
                                                      35854-86-5
    40228-18-0
                 56747-96-7
                             57500-00-2
                                          59094-77-8
                                                      62238-34-0
                             79869-58-2
    65505-17-1
                 76649-16-6
                                          93905-03-4
                                                      94280-80-5
    RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
        (flavorant, food consumption ratio of)
OS.CITING REF COUNT:
                             THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
                        2
                              (2 CITINGS)
ΤI
    Consumption ratio and food predominance of flavoring materials - second
    cumulative series
    Perfumer & Flavorist (
                                       1984), 9(4), 53-6, 58-9, 62, 65-72, 76-83
SO
    CODEN: PEFLDI; ISSN: 0361-8587
AΒ
    Detailed data are tabulated on the consumption ratio of food flavoring
    materials, i.e., the ratio between the quantity of a flavoring material
    consumed as an ingredient of food and the quantity of the same flavorant
    consumed as a component of added flavoring material. The food
```

1983. Of 347 flavoring materials covered, 296 were found as food predominant or those having the consumption ratio of >1; 205 of them had a consumption ratio of >10. ST flavoring material food diet ΙT Flavoring materials (food consumption ratio of) 57-11-4, biological studies ΙT 57-06-7 57-10-3, biological studies 60-12-8 60-33-3, biological studies 64-18-6, biological studies 67-63-0, biological studies 67-64-1, biological studies 71-23-8, biological studies 71-36-3, biological studies 74-93-1, biological studies biological studies 75-07-0, biological studies 75-18-3 76-49-3 78-70-6 78-83-1, biological studies 78-84-2 78-92-2 78-93-3, biological studies 78-98-8 79-09-4, 79-20-9 79-31-2 79-76-5 79-77-6 79-92-5 biological studies 80-71-7 83-34-1 87-44-5 90-02-8, biological studies 80-56-8 92-52-4, biological studies 90-05-1 90-12-0 93-15-2 93-16-3 93-51-6 93-58-3 93-89-0 94-46-2 95-48-7, biological studies 95-65-8 95-87-4 96-17-3 96-48-0 97-54-1 97-62-1 97-87-0 98-00-0 98-01-1, biological studies 98-02-2 98-55-5 98-85-1 98-86-2, biological studies 99-83-2 99-85-4 99-86-5 99-87-6 100-42-5, biological studies 100-51-6, biological studies 100-52-7biological studies 103-36-6 103-45-7 103-95-7 104-09-6 104-50-7 104-57-4 104-61-0 104-67-6 104-76-7 105-21-5 105-37-3 105-54-4 105-68-0 105-79-3 105-87-3 106-18-3 106-21-8 106-22-9 106-23-0 106-24-1 106-25-2 106-27-4 106-29-6 106-30-9 106-32-1 106-33-2 106-36-5 106-44-5, biological studies 106-70-7 107-85-7 106-35-4 107-87-9 107-92-6, biological studies 108-10-1 108-29-2 108 - 39 - 4, biological studies 108-50-9 108-64-5 108-95-2, biological studies 109-08-0 109-19-3 109-21-7 109-52-4, biological studies 109-60-4 109-94-4 109-97-7 110-19-0 110-38-3 110-39-4 110-43-0 110-62-3 110-93-0 110-86-1, biological studies 110-89-4, biological studies 111-11-5 111-13-7 111-27-3, biological studies 111-70-6 111-14-8 111-82-0 111-87-5, biological studies 112-05-0 112-06-1 112-12-9 112-14-1 112-17-4 112-30-1 112-31-2 112-54-9 112-37-8 112-80-1, biological studies 115-95-7 118-71-8 119-36-8 120 - 72 - 9biological studies 121-33-5 122-70-3 122-72-5 122-78-1 123-07-9 123-19-3 123-25-1 123-32-0 123-35-3 123-38-6, biological studies 123-51-3 123-66-0 123-72-8 123-75-1, biological studies 123-92-2 123-96-6 124-06-1 124-07-2, biological studies 124-10-7 124-13-0 124-19-6 127-41-3 127-91-3 138-87-4 140-11-4 140-26-1 140-88-5 141-12-8 141-14-0 141-16-2 141-78-6, biological studies 141-97-9 142-92-7 142-50-7 142-62-1, biological studies 143-07-7, biological 464 - 49 - 3studies 143-08-8 143-13-5 150-84-5 431-03-8 463-40-1 491-09-8 495-62-5 497-03-0 470-82-6 488-10-8 491-04-3 499-75-2 505-57-7 507-70-0 503-74-2 505-10-2 513-86-0 540-07-8 540-18-1 544-12-7 544-63-8, biological studies 542-55-2 543-49-7 546-79-2 547-63-7 556-82-1 556-24-1 557-48-2 562-74-3 576-26-1 586-62-9 582-24-1 589-38-8 589-98-0 590-01-2 590-86-3 592-84-7 600-14-6 593-08-8 606 - 45 - 1616-25-1 620-02-0 623-17-6 623-19-8 623-36-9 623-42-7 623-70-1 624-24-8 624-92-0 626-77-7 626-82-4 698-76-0 628-99-9 629-19-6 638-11-9 638-25-5 695-06-7 705-86-2 706-14-9 710-04-3 713-95-1 764-39-6 RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses) (flavorant, food consumption ratio of) ΙT 1117-52-8 821-55-6 823-22-3 870-23-5 1072-83-9 1117-55-1 1122-62-9 1124-11-4 1139-30-6 1192-62-7 1193-79-9 1365-19-1 1438-94-4 1632-73-1 2035-99-6 2050-01-3 2111-75-3 2198-61-0 2305-05-7 2305-21-7 2345-26-8 2349-07-7 2363-89-5 2412-80-8 2497-18-9 2639-63-6 2721-22-4 2463-53-8 2463-77-6 2785-89-9 3025-30-7 3142-66-3 3188-00-9 3268-49-3 3301-94-8 3391-86-4

consumption ratio was calculated from the USA literature data published after

```
3658-80-8
                            3777-69-3
    3658-77-3
                                      3796-70-1
                                                   3848-24-6
                                                               3913-71-1
    4411-89-6 4437-22-3
                           4630-07-3 4674-50-4 5392-40-5 5454-09-1
    5454-28-4 5457-70-5
                           5905-46-4 5905-47-5 5910-85-0 5910-89-4
                           6032-29-7 6290-37-5 6309-51-9
                                                             6378-65-0
    5989-27-5 6028-61-1
    6380-23-0 6789-80-6 6946-90-3 7452-79-1 7786-44-9 7786-61-0
    10032-15-2 13162-46-4 13327-56-5 13360-64-0
                                                      13360-65-1
    13532-18-8 13623-11-5 13679-46-4 13679-85-1 13925-00-3
               13925-07-0 13925-08-1 14667-55-1 15706-73-7
    13925-06-9
    15707-23-0 16409-46-4 17619-36-2 18640-74-9 18829-55-5
    21188-58-9 21834-92-4 22047-25-2 23328-62-3 23726-93-4
    24295-03-2 25152-84-5 29811-50-5 31501-11-8 35854-86-5
    40228-18-0 56747-96-7 57500-00-2 59094-77-8 62238-34-0
    65505-17-1 76649-16-6 79869-58-2
                                         93905-03-4 94280-80-5
    RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
        (flavorant, food consumption ratio of)
L29 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER:
                        1985:44486 HCAPLUS
DOCUMENT NUMBER:
                        102:44486
ORIGINAL REFERENCE NO.:
                        102:6987a,6990a
TITLE:
                        A case of artefact formation when using hydrogen as
                        carrier gas in capillary gas chromatography
                        Liddle, P. A. P.; Bossard, A.
AUTHOR(S):
                        Martini and Rossi, Saint-Ouen, 93401, Fr.
CORPORATE SOURCE:
SOURCE:
                        HRC & CC, Journal of High
Resolution Chromatography
                        and Chromatography Communications (1984), 7(11), 646-7
                        CODEN: HCJCDB; ISSN: 0344-7138
                        Journal
DOCUMENT TYPE:
LANGUAGE:
                        English
ABSTRACT:
A small amount (\leq 5\%) of anethole [104-46-1] was converted to
dihydroanethole [104-45-0] during its separation by gas chromatog. on a capillary
Carbowax 20M column with H as the carrier gas. The implications of this
finding for the determination of flavor volatiles by gas chromatog. are discussed.
    HRC & CC, Journal of High Resolution Chromatography and Chromatography
    Communications (1984), 7(11), 646-7
    CODEN: HCJCDB; ISSN: 0344-7138
    . . . a capillary Carbowax 20M column with H as the carrier gas. The
    implications of this finding for the determination of flavor volatiles by gas
    chromatog. are discussed.
    Hydrogenation
        (of anethole, in gas chromatog., flavor compound determination in
       relation to)
    104-45-0
    RL: FORM (Formation, nonpreparative)
        (formation of, in anethole determination by gas chromatog., flavor
       compound determination in relation to)
    104-46-1
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (hydrogenation of, in gas chromatog., flavor compound determination in
       relation to)
    HRC & CC, Journal of High Resolution Chromatography and Chromatography
    Communications (1984), 7(11), 646-7
    CODEN: HCJCDB; ISSN: 0344-7138
    A small amount (\leq 5%) of anethole [104-46-1] was converted to
    dihydroanethole [104-45-0] during its separation by gas chromatog. on a
    capillary Carbowax 20M column with {\tt H} as the carrier gas. The implications
    of this finding for the determination of flavor volatiles by gas chromatog. are
```

SO

AΒ

ΙT

ΤТ

ΙT

SO

AΒ

discussed.

IT Hydrogenation

(of anethole, in gas chromatog., flavor compound determination in relation to)

IT 104-45-0

RL: FORM (Formation, nonpreparative)

(formation of, in anethole determination by gas chromatog., flavor compound determination in relation to)

IT 104-46-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrogenation of, in gas chromatog., flavor compound determination in relation to)

L29 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1984:119500 HCAPLUS

DOCUMENT NUMBER: 100:119500

ORIGINAL REFERENCE NO.: 100:18161a, 18164a

TITLE: Study of artificial flavoring substances for

mutagenicity in the Salmonella/microsome, Basc and

micronucleus tests

AUTHOR(S): Wild, D.; King, M. T.; Gocke, E.; Eckhardt, K.

CORPORATE SOURCE: Zentrallab. Mutagenitaetspruef., Dtsch.

Forschungsgemeinsch., Freiburg, D-7800, Fed. Rep. Ger.

SOURCE: Food and Chemical Toxicology (1983), 21(6), 707-19

CODEN: FCTOD7; ISSN: 0278-6915

DOCUMENT TYPE: Journal LANGUAGE: English

ABSTRACT:

Seventy-six compds. used as artificial flavoring substances in food products were studied for mutagenic properties by the use of the Salmonella/mammalian microsome test (Ames test), Basc test on Drosophila melanogaster, and micronucleus test on mouse bone marrow. The following 4 compds. were mutagenic in Ames tests. EtNO2 [109-95-5], ethyl 3-phenylglycidate [121-39-1], 6-methylquinoline [91-62-3] and musk ambrette. Of these EtNO2 and musk ambrette also induced an increase in sex-linked recessive lethal mutations in Drosophila. Two further compds. ethyl 3-methyl-3-phenylglycidate [77-83-8] and 4-propylanisole [104-45-0], appeared weakly mutagenic in Drosophila only. The result with 4-propylanisole was of equivocal biol. significance. None of the flavoring substances induced micronuclei, i.e. cytogenetic damage in the bone marrow of mice.

- TI Study of artificial flavoring substances for mutagenicity in the Salmonella/microsome, Basc and micronucleus tests
- SO Food and Chemical Toxicology (1983), 21(6), 707-19 CODEN: FCTOD7; ISSN: 0278-6915
- AB Seventy-six compds. used as artificial flavoring substances in food products were studied for mutagenic properties by the use of the Salmonella/mammalian microsome test (Ames test), Basc. . . 4-propylanisole [104-45-0], appeared weakly mutagenic in Drosophila only. The result with 4-propylanisole was of equivocal biol. significance. None of the flavoring substances induced micronuclei, i.e. cytogenetic damage in the bone marrow of mice.
- ST flavoring material mutagenicity
- IT Mutagens

(flavoring materials)

IT Flavoring materials

(mutagenicity of)

IT 77-83-8 91-62-3 104-45-0 109-95-5 121-39-1

RL: ADV (Adverse effect, including toxicity); FFD (Food or feed use); BIOL (Biological study); USES (Uses)

(flavoring material, mutagenicity of)

OS.CITING REF COUNT: 62 THERE ARE 62 CAPLUS RECORDS THAT CITE THIS

RECORD (62 CITINGS)

- TI Study of artificial flavoring substances for mutagenicity in the Salmonella/microsome, Basc and micronucleus tests
- SO Food and Chemical Toxicology (1983), 21(6), 707-19 CODEN: FCTOD7; ISSN: 0278-6915
- AB Seventy-six compds. used as artificial flavoring substances in food products were studied for mutagenic properties by the use of the Salmonella/mammalian microsome test (Ames test), Basc test on Drosophila melanogaster, and micronucleus test on mouse bone marrow. The following 4 compds. were mutagenic in Ames tests. EtNO2 [109-95-5], ethyl 3-phenylglycidate [121-39-1], 6-methylquinoline [91-62-3] and musk ambrette. Of these EtNO2 and musk ambrette also induced an increase in sex-linked recessive lethal mutations in Drosophila. Two further compds. ethyl 3-methyl-3-phenylglycidate [77-83-8] and 4-propylanisole [104-45-0], appeared weakly mutagenic in Drosophila only. The result with 4-propylanisole was of equivocal biol. significance. None of the flavoring substances induced micronuclei, i.e. cytogenetic damage in the bone marrow of mice.
- ST flavoring material mutagenicity
- IT Mutagens

(flavoring materials)

IT Flavoring materials

(mutagenicity of)

L29 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1983:538318 HCAPLUS

DOCUMENT NUMBER: 99:138318

ORIGINAL REFERENCE NO.: 99:21245a,21248a

TITLE: Volatile flavor components of dried bonito (Katsuobushi). II. From the neutral fraction

AUTHOR(S): Yajima, Izumi; Nakamura, Mikio; Sakakibara, Hidemasa;

Ide, Junichi; Yanai, Tetsuya; Hayashi, Kazuo

CORPORATE SOURCE: Kawasaki Res. Lab., T. Hasegawa Co. Ltd., Kawasaki,

211, Japan

SOURCE: Agricultural and Biological Chemistry (1983), 47(8),

1755-60

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal LANGUAGE: English

ABSTRACT:

The aqueous extract of dried bonito (Katsuobushi) was distilled under reduced pressure.

The resulting distillate was extracted with Et20 and the extract was separated into acidic, phenolic, basic, and neutral fractions. The neutral fraction was further fractionated into 10 subfractions by silica gel column chromatog. All these subfractions were analyzed by gas chromatog. and gas chromatog.—mass spectrometry. One hundred and sixty-five compds. were identified and 12 compds. were tentatively identified from the neutral fraction. Among them, 111 compds. were newly identified as flavor components of Katsuobushi.

- TI Volatile flavor components of dried bonito (Katsuobushi). II. From the neutral fraction
- SO Agricultural and Biological Chemistry (1983), 47(8), 1755-60 CODEN: ABCHA6; ISSN: 0002-1369
- AB . . . were identified and 12 compds. were tentatively identified from the neutral fraction. Among them, 111 compds. were newly identified as flavor components of Katsuobushi.

```
ST
    bonito flavor volatile substance
ΤТ
    Bonito
        (dried, volatile compds. of, flavor in relation to)
    Volatile substances
ΙT
    Alcohols, biological studies
    Esters, biological studies
    Ethers, biological studies
    Hydrocarbons, biological studies
    Ketones, biological studies
    Lactones
    RL: BIOL (Biological study)
       (of dried bonito, flavor in relation to)
ΙT
    Flavor
        (volatiles, of dried bonito)
ΙT
            64-17-5, biological studies
                                           66-25-1
                                                    71-36-3, biological
    60 - 12 - 8
    studies
              71-41-0, biological studies
                                           76-22-2 77-53-2
                                                              78-70-6
    78-92-2
              80-71-7
                      83-33-0
                                83-34-1
                                           89-71-4
                                                   89-74-7
                                                              90-12-0
             91-20-3, biological studies
                                                   92-52-4, biological
    91-16-7
                                           91-57-6
              93-04-9
                      93-55-0 93-58-3
                                           94-59-7
                                                   95-13-6
    studies
                                                             96-41-3
              98-01-1, biological studies
    98-00-0
                                          98-55-5
                                                   98-86-2, biological
    studies
              100-47-0, biological studies
                                           100-51-6, biological studies
    100-52-7, biological studies
                                 100-84-5
                                            104-45-0
                                                       104-55-2
                        108-88-3, biological studies
    104-87-0
               106-68-3
                                                       108-94-1, biological
    studies
              109-94-4
                         109-97-7
                                   110-43-0 110-62-3
                                                        110-93-0
                                                                   111-13-7
    111-27-3, biological studies 111-70-6
                                             111-71-7
                                                       112-12-9
                                                                  112-31-2
    112-40-3
              112-95-8 120-58-1 120-72-9, biological studies
                                                                  120-92-3
              122-03-2
    122-00-9
                         122-78-1
                                   123-51-3
                                              124-13-0
                                                         124-18-5
                                                                    124-19-6
    137-32-6
              140-29-4 141-78-6, biological studies 271-89-6 470-82-6
              483-76-1 483-77-2 487-12-7
    481-34-5
                                             494-99-5 507-70-0
                                                                  542-54-1
                                              590-86-3
    544-76-3
              577-16-2 589-55-9 589-98-0
                                                        593-45-3
                                                                   593-49-7
    600-14-6 616-25-1 623-17-6 626-93-7 629-50-5
                                                        629-59-4
                                                                   629-62-9
    629-78-7 629-80-1 629-92-5 629-94-7
                                             629-97-0
                                                         629-99-2
                                                                   630-01-3
    630-02-4 630-03-5 634-36-6 638-67-5
                                             645-13-6
                                                        646-31-1
                                                                    693-54-9
    706-14-9
              821-55-6 928-95-0 930-30-3 930-68-7 1072-83-9
    1120-21-4 1120-72-5 1120-73-6 1121-05-7 1121-18-2 1192-62-7
    1193-18-6 1193-79-9
                          1197-01-9
                                      1334-76-5
                                                 1575-46-8 1576-87-0
    1576 - 96 - 1 \qquad 1679 - 49 - 8 \qquad 1757 - 42 - 2 \qquad 2345 - 28 - 0 \qquad 2548 - 87 - 0 \qquad 2758 - 18 - 1
    3131-63-3 3188-00-9 3391-86-4
                                      3796-70-1 4041-11-6
                                                              4265-25-2
    4313-02-4 4313-03-5 5337-93-9
                                      5577-44-6
                                                5888-51-7
                                                              5888-52-8
    6380-23-0 6443-69-2 6728-26-3 6728-31-0 10547-84-9 13400-02-7
    14963-40-7 18409-17-1 18787-63-8 18829-56-6
                                                      23033-96-7
    23048-13-7
               25152-83-4 25152-84-5
                                        25586-39-4 26370-28-5
    28790-86-5
               29036-25-7 30434-64-1
                                         32142-08-8 33488-51-6
    35389-48-1
                38743-20-3 41564-88-9
                                         50306-18-8
                                                      56438-71-2
    56722-23-7
                 57643-02-4
                            62019-23-2
                                          72692-71-8 79379-60-5
                 87259-53-8
                            87305-48-4
    87259-01-6
    RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
    BIOL (Biological study); OCCU (Occurrence)
        (of bonito, flavor in relation to)
OS.CITING REF COUNT:
                             THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
                       7
                              (7 CITINGS)
    Volatile flavor components of dried bonito (Katsuobushi). II. From the
ΤI
    neutral fraction
SO
    Agricultural and Biological Chemistry (1983), 47(8), 1755-60
    CODEN: ABCHA6; ISSN: 0002-1369
    The aqueous extract of dried bonito (Katsuobushi) was distilled under reduced
    pressure. The resulting distillate was extracted with Et20 and the extract was
    separated into acidic, phenolic, basic, and neutral fractions. The neutral
    fraction was further fractionated into 10 subfractions by silica gel
    column chromatog. All these subfractions were analyzed by gas chromatog.
    and gas chromatog.-mass spectrometry. One hundred and sixty-five compds.
```

```
neutral fraction. Among them, 111 compds. were newly identified as
    flavor components of Katsuobushi.
    bonito flavor volatile substance
ST
ΤТ
    Bonito
       (dried, volatile compds. of, flavor in relation to)
ΙT
    Volatile substances
    Alcohols, biological studies
    Esters, biological studies
    Ethers, biological studies
    Hydrocarbons, biological studies
    Ketones, biological studies
    Lactones
    RL: BIOL (Biological study)
       (of dried bonito, flavor in relation to)
ΙT
    Flavor
       (volatiles, of dried bonito)
ΙT
    60-12-8
              64-17-5, biological studies
                                          66-25-1
                                                   71-36-3, biological
              71-41-0, biological studies
                                          76-22-2
                                                    77-53-2
                                                            78-70-6
    studies
              80-71-7
    78-92-2
                      83-33-0
                                83-34-1
                                          89-71-4
                                                  89-74-7
                                                             90-12-0
             91-20-3, biological studies
    91-16-7
                                          91-57-6
                                                   92-52-4, biological
    studies
              93-04-9
                      93-55-0
                               93-58-3
                                          94-59-7
                                                    95-13-6
                                                            96-41-3
              98-01-1, biological studies
                                                  98-86-2, biological
    98-00-0
                                          98-55-5
    studies
                                          100-51-6, biological studies
              100-47-0, biological studies
    100-52-7, biological studies
                                100-84-5
                                           104-45-0
                                                      104-55-2
                                                      108-94-1, biological
    104-87-0
              106-68-3
                        108-88-3, biological studies
              109-94-4
                        109-97-7
                                  110-43-0 110-62-3
                                                      110-93-0
    studies
                                                                 111-13-7
                                           111-71-7
    111-27-3, biological studies 111-70-6
                                                      112-12-9
                                                                 112-31-2
    112-40-3
              112-95-8 120-58-1 120-72-9, biological studies
                                                                 120-92-3
                                                       124-18-5
    122-00-9
              122-03-2 122-78-1
                                  123-51-3
                                             124-13-0
                                                                  124-19-6
    137-32-6
             140-29-4 141-78-6, biological studies 271-89-6 470-82-6
    481-34-5
              483-76-1 483-77-2 487-12-7 494-99-5 507-70-0 542-54-1
    544-76-3 577-16-2 589-55-9 589-98-0
                                             590-86-3
                                                       593-45-3
                                                                  593-49-7
    600-14-6 616-25-1 623-17-6 626-93-7 629-50-5
                                                       629-59-4
                                                                  629-62-9
    629-78-7
              629-80-1 629-92-5 629-94-7 629-97-0
                                                       629-99-2
                                                                  630-01-3
                                                                   693-54-9
    630-02-4
              630-03-5 634-36-6 638-67-5 645-13-6
                                                       646-31-1
                        928-95-0 930-30-3 930-68-7 1072-83-9
    706-14-9
              821-55-6
    1120-21-4
              1120-72-5
                         1120-73-6 1121-05-7 1121-18-2 1192-62-7
    1193-18-6
              1193-79-9
                          1197-01-9
                                     1334-76-5 1575-46-8
                                                           1576-87-0
    1576-96-1 1679-49-8
                         1757-42-2
                                     2345-28-0 2548-87-0
                                                           2758-18-1
              3188-00-9 3391-86-4
                                     3796-70-1 4041-11-6
    3131-63-3
                                                            4265-25-2
    4313-02-4
              4313-03-5 5337-93-9
                                     5577-44-6
                                                5888-51-7
                                                             5888-52-8
                           6728-26-3 6728-31-0 10547-84-9 13400-02-7
    6380-23-0
              6443-69-2
    14963-40-7
               18409-17-1 18787-63-8 18829-56-6
                                                     23033-96-7
    23048-13-7
                                        25586-39-4
                25152-83-4
                           25152-84-5
                                                     26370-28-5
                                         32142-08-8
    28790-86-5
                29036-25-7
                           30434-64-1
                                                    33488-51-6
                           41564-88-9
    35389-48-1
                38743-20-3
                                         50306-18-8 56438-71-2
                                         72692-71-8
    56722-23-7
                                                     79379-60-5
                57643-02-4
                            62019-23-2
                           87305-48-4
    87259-01-6
                87259-53-8
    RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
    BIOL (Biological study); OCCU (Occurrence)
       (of bonito, flavor in relation to)
L29 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER:
                       1983:468991 HCAPLUS
DOCUMENT NUMBER:
                       99:68991
ORIGINAL REFERENCE NO.: 99:10709a,10712a
TITLE:
                       The metabolism of p-propylanisole in the rat and mouse
                       and its variation with dose
AUTHOR(S):
                       Sangster, S. A.; Caldwell, J.; Hutt, A. J.; Smith, R.
                       L.
```

were identified and 12 compds. were tentatively identified from the

CORPORATE SOURCE: Dep. Pharmacol., St. Mary's Hosp. Med. Sch., London,

W2 1PG, UK

SOURCE: Food and Chemical Toxicology (1983), 21(3), 263-71

CODEN: FCTOD7; ISSN: 0278-6915

DOCUMENT TYPE: Journal LANGUAGE: English

ABSTRACT:

The metabolism of the synthetic flavoring, p-propylanisole [104-45-0], was studied in rats and mice and the variation in its metabolism with dose was determined

[Methoxy-14C]-p-propylanisole was given to female Wistar albino rats orally and male CD-1 mice i.p. at doses ranging from 0.05 to 1500 mg/kg body weight (0.2-20 $\mu\text{Ci/animal})$. The urine, feces, and 14CO2 in the expired air were collected. The urinary metabolites were separated by solvent extraction, TLC, and high-pressure liquid chromatog., and characterized by mass and NMR spectroscopy and comparison with authentic samples. Three major 14C-labeled urinary metabolites were excreted, 1'- [5349-60-0] and 2'-hydroxy-p-propylanisole [30314-64-8] and p-methoxyhippuric acid [13214-64-7]; 14CO2 was eliminated in the expired air, arising from oxidative O-demethylation. The relative quantities of the metabolites varied markedly with dose. The percentage of the dose that was O-demethylated fell as the dose increased and the proportion in the form of urinary metabolites increased. The relative proportions of the major urinary metabolites also changed with dose. In view of the great discrepancy between human exposure to p-propylanisole in foods (.apprx.15 $\mu g/day$) and the doses used for its toxicol. evaluation in animals, these results emphasize the importance of considering dose-dependent metabolism when interpreting the significance for man of animal data obtained at very high doses.

- SO Food and Chemical Toxicology (1983), 21(3), 263-71 CODEN: FCTOD7; ISSN: 0278-6915
- AB The metabolism of the synthetic flavoring, p-propylanisole [104-45-0], was studied in rats and mice and the variation in its metabolism with dose was determined [Methoxy-14C]-p-propylanisole was given to. . .
- ST propylanisole flavoring toxicity metab rat
- IT Air, respiratory

Feces

Urine

(p-propylanisole food flavoring metabolites in, toxicity in relation to)

IT Flavoring materials

(p-propylanisole, metabolism of, in rats and mice, toxicity in relation to) 104-45-0

RL: BIOL (Biological study)

(flavoring material, metabolism of, in rats and mice, toxicity in relation to)

IT 5349-60-0

ΙT

RL: BIOL (Biological study)

(p-propylanisol flavoring material metabolite, in rats and mice, toxicity in relation to)

IT 13214-64-7 30314-64-8

RL: BIOL (Biological study)

- OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
- SO Food and Chemical Toxicology (1983), 21(3), 263-71 CODEN: FCTOD7; ISSN: 0278-6915
- AB The metabolism of the synthetic flavoring, p-propylanisole [104-45-0], was studied in rats and mice and the variation in its metabolism with dose was determined [Methoxy-14C]-p-propylanisole was given to female Wistar albino rats orally and male CD-1 mice i.p. at doses ranging from 0.05 to 1500

mg/kg body weight (0.2-20 μ Ci/animal). The urine, feces, and 14CO2 in the expired air were collected. The urinary metabolites were separated by solvent extraction, TLC, and high-pressure liquid chromatog., and characterized by mass and NMR spectroscopy and comparison with authentic samples. Three major 14C-labeled urinary metabolites were excreted, 1'- [5349-60-0] and 2'-hydroxy-p-propylanisole [30314-64-8] and p-methoxyhippuric acid [13214-64-7]; 14CO2 was eliminated in the expired air, arising from oxidative O-demethylation. The relative quantities of the metabolites varied markedly with dose. The percentage of the dose that was O-demethylated fell as the dose increased and the proportion in the form of urinary metabolites increased. The relative proportions of the major urinary metabolites also changed with dose. In view of the great discrepancy between human exposure to p-propylanisole in foods (.apprx.15 $\mu g/day$) and the doses used for its toxicol. evaluation in animals, these results emphasize the importance of considering dose-dependent metabolism when interpreting the significance for man of animal data obtained at very high doses. propylanisole flavoring toxicity metab rat Air, respiratory Feces Urine (p-propylanisole food flavoring metabolites in, toxicity in relation to) Flavoring materials (p-propylanisole, metabolism of, in rats and mice, toxicity in relation to) 104-45-0 RL: BIOL (Biological study) (flavoring material, metabolism of, in rats and mice, toxicity in relation to) 5349-60-0 RL: BIOL (Biological study) (p-propylanisol flavoring material metabolite, in rats and mice, toxicity in relation to) 13214-64-7 30314-64-8 RL: BIOL (Biological study) (p-propylanisole flavoring material metabolite, in rats and mice, toxicity in relation to) L29 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN 1978:103450 HCAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 88:103450

ORIGINAL REFERENCE NO.: 88:16217a,16220a

TITLE: Occurrence of sesquiterpenes in mountain cheese

volatiles

Dumont, Jean Pierre; Adda, Jacques AUTHOR(S):

Lab. Technol. Laitiere, Inst. Natl. Rech. Agron., CORPORATE SOURCE:

Jouy-en-Josas, Fr.

SOURCE: Journal of Agricultural and Food Chemistry (1978),

26(2), 364-7

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal LANGUAGE: English

ABSTRACT:

ST

ΙT

ΙT

ΙT

ΙT

TТ

Gas chromatog.-mass spectrometry of Beaufort cheese volatiles has led to the identification of 140 components including 9 sesquiterpenes. Sesquiterpenes were only found in cheeses made from summer milk when cows were grazing on high-altitude pastures. The effect of the traditional ripening process on volatile flavor compds. is also discussed.

Journal of Agricultural and Food Chemistry (1978), 26(2), 364-7 SO CODEN: JAFCAU; ISSN: 0021-8561

```
. . . made from summer milk when cows were grazing on high-altitude
AΒ
    pastures. The effect of the traditional ripening process on volatile
    flavor compds. is also discussed.
    Hydrocarbons, biological studies
ΙT
    Sesquiterpenes and Sesquiterpenoids
    RL: BIOL (Biological study)
        (of cheese flavor)
              64-17-5, biological studies
                                           66-25-1
                                                     71-23-8, biological
ΙT
    60-12-8
    studies
             71-36-3, biological studies 71-41-0, biological studies
    71-43-2, biological studies
                                 74-93-1, biological studies
    78-83-1, biological studies 78-92-2 78-93-3, biological studies
             91-20-3, biological studies
                                           93-58-3
                                                     95-16-9
    98-01-1, biological studies
                                98-82-8 98-85-1 98-86-2, biological
    studies
             100-41-4, biological studies 100-42-5, biological studies
    100-51-6, biological studies 100-52-7, biological studies 103-45-7
    105-37-3
               105-46-4
                         105-54-4
                                   105-66-8
                                              105-68-0
                                                         106-32-1
                                                                     106-68-3
    107-87-9
                         108-88-3, biological studies 108-95-2, biological
               108-64-5
             109-60-4 110-38-3
                                    110-42-9 110-43-0
                                                        110-62-3 110-86-1,
    studies
                        111-13-7
                                    111-27-3, biological studies
                                                                 111-65-9,
    biological studies
                        111-71-7
                                    111-84-2
                                              111-87-5, biological studies
    biological studies
                        120-72-9, biological studies
    112-12-9
              112-40-3
                                                       123-51-3
                                                                  123-66-0
                                               124-18-5
    123-86-4
               123-92-2
                          123-96-6 124-13-0
                                                          124-19-6
                                                                     138-86-3
    141-78-6, biological studies 151-10-0 473-55-2
                                                       505-10-2
               543-49-7 556-24-1
                                    565-61-7
    513-86-0
                                               590-86-3
                                                          591-78-6
                                                                     593-08-8
    624-54-4
               624-92-0
                          626-93-7
                                    628-99-9
                                               629-50-5
                                                          629-62-9
                                                                     644 - 49 - 5
    693-54-9
               705-86-2
                          706-14-9
                                     713-95-1
                                               819-97-6
                                                          821-55-6
    1067-20-5
                1120-21-4
                           1319-77-3
                                      1321-94-4
                                                   1330-20-7, biological
    studies 1534-08-3 1618-26-4 1653-30-1 2198-61-0 3268-49-3
    3391-86-4
               3658-80-8
                          5870-68-8 6032-29-7
                                                  7452-79-1
                                                               7783-06-4,
    biological studies 25429-37-2 25550-14-5
                                                  25704-73-8
                                                               27936-13-6
    28473-21-4
               28804-88-8
                             29224-55-3
                                         29611-84-5
                                                       42474-44-2
                 61193-19-9
                              63335-87-5
    53535-33-4
                                         63335-88-6
                                                       65436-56-8
    RL: BIOL (Biological study)
        (of cheese flavor)
OS.CITING REF COUNT:
                        52
                              THERE ARE 52 CAPLUS RECORDS THAT CITE THIS
                              RECORD (52 CITINGS)
SO
    Journal of Agricultural and Food Chemistry (1978), 26(2), 364-7
    CODEN: JAFCAU; ISSN: 0021-8561
AΒ
    Gas chromatog.-mass spectrometry of Beaufort cheese volatiles has led to
    the identification of 140 components including 9 sesquiterpenes.
    Sesquiterpenes were only found in cheeses made from summer milk when cows
    were grazing on high-altitude pastures. The effect of the traditional
    ripening process on volatile flavor compds. is also discussed.
    Hydrocarbons, biological studies
ΙT
    Sesquiterpenes and Sesquiterpenoids
    RL: BIOL (Biological study)
        (of cheese flavor)
    60-12-8
              64-17-5, biological studies
                                                     71-23-8, biological
ΙT
                                           66-25-1
              71-36-3, biological studies
                                          71-41-0, biological studies
    studies
    71-43-2, biological studies 74-93-1, biological studies
                                                               75-18-3
                                 78-92-2
    78-83-1, biological studies
                                           78-93-3, biological studies
              91-20-3, biological studies
    83-34-1
                                           93-58-3
                                                     95-16-9
                                                               96-17-3
    98-01-1, biological studies 98-82-8
                                           98-85-1
                                                     98-86-2, biological
    studies 100-41-4, biological studies 100-42-5, biological 100-51-6, biological studies 100-52-7, biological studies
                                            100-42-5, biological studies
                                                                103-45-7
                                   105-66-8
                                               105-68-0
                                                          106-32-1
    105-37-3
              105-46-4
                         105-54-4
                                                                    106-68-3
    107-87-9
               108-64-5
                         108-88-3, biological studies 108-95-2, biological
    studies 109-60-4 110-38-3
                                                        110-62-3 110-86-1,
                                   110-42-9 110-43-0
    biological studies 111-13-7 111-27-3, biological studies 111-65-9,
    biological studies 111-71-7 111-84-2 111-87-5, biological studies
    112-12-9 112-40-3 120-72-9, biological studies 123-51-3 123-66-0
```

123-86-4 123-92-2 123-96-6 124-13-0 124-18-5 124-19-6 138 - 86 - 3141-78-6, biological studies 151-10-0 473-55-2 505-10-2 513-86-0 543-49-7 556-24-1 565-61-7 590-86-3 591-78-6 593-08-8 624-54-4 624-92-0 626-93-7 628-99-9 629-50-5 629-62-9644 - 49 - 5693-54-9 705-86-2 706-14-9 713-95-1 819-97-6 821-55-61067-20-5 1120-21-4 1319-77-3 1321-94-4 1330-20-7, biological studies 1534-08-3 1618-26-4 1653-30-1 2198-61-0 3268-49-3 3391-86-4 3658-80-8 5870-68-8 6032-29-7 7452-79-1 7783-06-4, biological studies 25429-37-2 25550-14-5 25704-73-8 27936-13-6 28473-21-4 28804-88-8 29224-55-3 29611-84-5 42474-44-2 53535-33-4 61193-19-9 63335-87-5 63335-88-6 65436-56-8 RL: BIOL (Biological study)

(of cheese flavor)

L29 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

1976:574492 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 85:174492

ORIGINAL REFERENCE NO.: 85:27889a,27892a

Heterocyclic flavoring compositions for tobacco TITLE: INVENTOR(S): Pittet, Alan O.; Pascale, John V.; Hruza, Denis E. PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA U.S., 14 pp. Continuation-in-part of U.S. 3,869,554. SOURCE:

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3980089	A	19760914	US 1974-468180	19740508 <
US 3869554	A	19750304	US 1972-246484	19720421 <
CA 1016737	A1	19770906	CA 1973-163010	19730206 <
AU 7352088	A	19740815	AU 1973-52088	19730212 <
CH 566722	A5	19750930	СН 1973-3608	19730313 <
BE 796761	A1	19730914	BE 1973-128787	19730314 <
JP 49014668	A	19740208	JP 1973-29552	19730315 <
FR 2201838	A1	19740503	FR 1973-9410	19730315 <
GB 1414677	A	19751119	GB 1973-19282	19730424 <
PRIORITY APPLN. INFO.:			US 1972-246484	A2 19720421
GRAPHIC IMAGE:				

ABSTRACT:

Addition of >1 N-substituted pyrroles (I) (R1 = R2 = H or alkyl; R3 = alkyl, alkenyl, cycloalkyl, phenalkyl, carboalkoxyalkyl, alkoxyphenylalkyl, hydroxyalkyl, alkoxyalkyl, (alkylthio)alkyl, mercaptoalkyl, mercaptophenyl, pyrazinyl, pyridinyl, or thiazolyl) improved the flavor and aroma of tobacco products. Two hundred ml glacial AcOH was added dropwise to a mixture of 2-aminopyrazine 43 and 2,5-dimethoxytetrahydrofuran 66 g at 20°. The mixture was refluxed at $105\,^{\circ}$ for $30\,^{\circ}$ min and, after cooling, was made basic with 325 ml of 30% NaOH and steam-distilled The distillate was worked up to obtain 51.3 g N-(2-pyrazinyl)pyrrole (I, R1 = R2 = H, R3 = 2-pyrazinyl) (II). The following mixture was prepared; fenugreek extract 20.00, valerian oil 7.00, dimethylresorcinol 0.25, propylene glycol 39.75, II 3.00, and water 10.00 parts. The mixture, when added to tobacco to 0.10-0.70%, imparted a nutty pyrrazinelike odor to the tobacco and confered a walnut character on the product.

```
Heterocyclic flavoring compositions for tobacco
ΤI
PΙ
      US 3980089 19760914
                         KIND DATE
                             KIND DATE APPLICATION NO. DATE
      PATENT NO.
     US 3980089 A 19760914 US 1974-468180 19740508 <--
US 3869554 A 19750304 US 1972-246484 19720421 <--
CA 1016737 A1 19770906 CA 1973-163010 19730206 <--
AU 7352088 A 19740815 AU 1973-52088 19730212 <--
CH 566722 A5 19750930 CH 1973-3608 19730313 <--
BE 796761 A1 19730914 BE 1973-128787 19730314 <--
JP 49014668 A 19740208 JP 1973-29552 19730315 <--
FR 2201838 A1 19740503 FR 1973-9410 19730315 <--
GB 1414677 A 19751119 GB 1973-19282 19730424 <--
      . . . alkyl; R3 = alkyl, alkenyl, cycloalkyl, phenalkyl, carboalkoxyalkyl, alkoxyphenylalkyl, hydroxyalkyl, alkoxyalkyl,
AΒ
      (alkylthio)alkyl, mercaptoalkyl, mercaptophenyl, pyrazinyl, pyridinyl, or
      thiazolyl) improved the flavor and aroma of tobacco products. Two
      hundred ml glacial AcOH was added dropwise to a mixture of 2-aminopyrazine
      43 and. . .
      tobacco flavor arom compn; pyrrole tobacco flavor aroma;
ST
      pyrazinylpyrrole tobacco flavor aroma
ΙT
      Tobacco
       (aroma and flavor of, N-substituted pyrrole improvement of)
      57-55-6, biological studies 109-97-7D, 1H-Pyrrole, derivs.
ΤТ
      151-10-0
      RL: BIOL (Biological study)
         (for tobacco aroma and flavor improvement)
      5044-41-7P 6719-02-4P 31708-14-2P 50463-83-7P 50966-64-8P
ΙT
      50966-65-9P 50966-66-0P 50966-67-1P 50966-68-2P 50966-70-6P
      50966-71-7P 50966-72-8P 50966-73-9P 50966-74-0P 50966-75-1P
      50966-76-2P 50966-79-5P
      RL: PREP (Preparation)
         (preparation and tobacco aroma and flavor improvement by)
ΙT
      RL: BIOL (Biological study)
          (prepn.and tobacco aroma and flavor improvement by)
ΙT
      2051-97-0 7435-07-6 23694-49-7
      RL: BIOL (Biological study)
          (tobacco aroma and flavor improvement by)
OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
```

TI Heterocyclic flavoring compositions f	or t	obacco
--	------	--------

ΡI	US	3980089	19760914

PAT	TENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US	3980089	A	19760914	US 1974-468180	19740508 <
US	3869554	A	19750304	US 1972-246484	19720421 <
CA	1016737	A1	19770906	CA 1973-163010	19730206 <
AU	7352088	A	19740815	AU 1973-52088	19730212 <
СН	566722	A5	19750930	CH 1973-3608	19730313 <
BE	796761	A1	19730914	BE 1973-128787	19730314 <
JP	49014668	A	19740208	JP 1973-29552	19730315 <
FR	2201838	A1	19740503	FR 1973-9410	19730315 <
GB	1414677	A	19751119	GB 1973-19282	19730424 <

(6 CITINGS)

Addition of >1 N-substituted pyrroles (I) (R1 = R2 = H or alkyl; R3 = alkyl, AΒ alkenyl, cycloalkyl, phenalkyl, carboalkoxyalkyl, alkoxyphenylalkyl, hydroxyalkyl, alkoxyalkyl, (alkylthio)alkyl, mercaptoalkyl, mercaptophenyl, pyrazinyl, pyridinyl, or thiazolyl) improved the flavor and aroma of tobacco products. Two hundred ml glacial AcOH was added dropwise to a mixture of 2-aminopyrazine 43 and 2,5-dimethoxytetrahydrofuran 66 g at 20° . The mixture was refluxed at 105° for 30 min and, after cooling, was made basic with 325 ml of 30% NaOH and steam-distilled The distillate was worked up to obtain 51.3 g N-(2-pyrazinyl) pyrrole (I, R1 = R2 = H, R3 = 2-pyrazinyl) (II). The following mixture was prepared; fenugreek extract 20.00, valerian oil 7.00, dimethylresorcinol 0.25, propylene glycol 39.75, II 3.00, and water 10.00 parts. The mixture, when added to tobacco to 0.10-0.70%, imparted a nutty pyrrazinelike odor to the tobacco and confered a walnut character on the product. ST tobacco flavor arom compn; pyrrole tobacco flavor aroma; pyrazinylpyrrole tobacco flavor aroma ΙT Tobacco (aroma and flavor of, N-substituted pyrrole improvement of) 57-55-6, biological studies 109-97-7D, 1H-Pyrrole, derivs. ΤТ 151-10-0 RL: BIOL (Biological study) (for tobacco aroma and flavor improvement) ΙT 5044-41-7P 6719-02-4P 31708-14-2P 50463-83-7P 50966-64-8P 50966-65-9P 50966-66-0P 50966-67-1P 50966-68-2P 50966-70-6P 50966-71-7P 50966-72-8P 50966-73-9P 50966-74-0P 50966-75-1P

50966-76-2P 50966-79-5P

RL: PREP (Preparation)

(preparation and tobacco aroma and flavor improvement by)

ΙT 50966-77-3

RL: BIOL (Biological study)

(prepn.and tobacco aroma and flavor improvement by)

7435-07-6 23694-49-7 ΤТ 2051-97-0

RL: BIOL (Biological study)

(tobacco aroma and flavor improvement by)

L29 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1976:419413 HCAPLUS

DOCUMENT NUMBER: 85:19413 ORIGINAL REFERENCE NO.: 85:3173a,3176a TITLE: Flavoring agent

INVENTOR(S): Winter, Max; Gautschi, Fritz; Flament, Ivon; Stoll,

> Max; Goldman, Irving M. Firmenich S. A., Switz.

U.S., 8 pp. SOURCE:

CODEN: USXXAM DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 31

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3947603	A	19760330	US 1974-482686	19740624 <
BR 6679143	D0	19730911	BR 1966-179143	19660429 <
СН 566111	A5	19750915	CH 1970-13417	19660429 <
GB 1156487	A	19690625	GB 1966-1156487	19660502 <
NO 134890	В	19760927	NO 1968-108	19680110 <
NO 134891	В	19760927	NO 1968-1709	19680502 <
NO 134892	В	19760927	NO 1968-1710	19680502 <
NO 134893	В	19760927	NO 1968-1711	19680502 <
NO 134240	В	19760531	NO 1969-5184	19691231 <

NC	134894	В	19760927	NO	1969-5180		19691231 <
	134895	В	19760927		1969-5181		19691231 <
	134896	В	19760927		1969-5183		19691231 <
	3702253	A	19721107		1970-70560		19700908 <
JP	50004736	В	19750224	JР	1971-19574		19710330 <
US	4303689	A	19811201	US	1972-243850		19720413 <
DK	139374	В	19790212	DK	1973-5432		19731005 <
DK	139374	С	19790716				
DK	139454	В	19790226	DK	1973-5428		19731005 <
DK	7 139454	С	19790813				
DK	7 139553	В	19790312	DK	1973-5429		19731005 <
DK	7 139553	С	19790903				
DK	7 139551	В	19790312	DK	1973-5430		19731005 <
DK	139551	С	19790903				
DK	7 139552	В	19790312	DK	1973-5431		19731005 <
	139552	С	19790827				
	7 139605	В	19790319	DK	1973-5426		19731005 <
DK	7 139605	С	19790903				
	140243	В	19790716	DK	1973-5427		19731005 <
	140243	С	19791203				
	7 140361	В	19790813	DK	1973-5433		19731005 <
	7 140361	С	19800114				
	7 140362	В	19790813	DK	1973-5434		19731005 <
	140362	С	19800114				
	3900582	A	19750819		1974-482818		19740624 <
PRIORIT	Y APPLN. INFO.:				1965-452342		19650430
					1966-543069		19660418
					1970-70560		19700908
					1972-243866		19720413
					1965-542342	А	19650430
					1965-543069	A	19650430
					1966-2217	A	19660429
7 D C T D 7 C				ИО	1966-162820	А	19660429

ABSTRACT:

Phenolic compds. enhancing or altering the flavor of beverages made from soluble coffee are described. Flavor characteristics in sirup of coffee bases are tabulated for: 2-ethylphenol [90-00-6], 3-ethylphenol [620-17-7], 4-ethylphenol [123-07-9], 4-isopropylphenol [99-89-8], 2,3-xylenol [526-75-0], 2,4-xylenol [105-67-9], 2,5-xylenol [95-87-4], 2,6-xylenol [576-26-1], 3,4-xylenol [95-65-8], 3,5-xylenol [108-68-9], 2-hydroxyacetophenone [582-24-1], 2-hydroxypropiophenone [610-99-1], 4-hydroxypropiophenone [70-70-2], 5-methyl-2-hydroxyacetophenone [1450-72-2], 2,3,5-trimethylphenol [697-82-5], 2,4,6-trimethylphenol [527-60-6], 2,4,5-trimethylphenol [496-78-6], 3,4,5-trimethylphenol [527-54-8], 4-ethyl-2-methoxyphenol [2785-89-9], 4-propyl-2-methoxyphenol [2785-87-7], and 4-vinyl-1,2-dimethoxybenzene [6380-23-0].

TI Flavoring agent

PI US 3947603 19760330

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	US 3947603 BR 6679143 CH 566111 GB 1156487 NO 134890 NO 134891 NO 134892 NO 134893 NO 134240	A D0 A5 A B B B B	19760330 19730911 19750915 19690625 19760927 19760927 19760927 19760531	US 1974-482686 BR 1966-179143 CH 1970-13417 GB 1966-1156487 NO 1968-108 NO 1968-1709 NO 1968-1710 NO 1968-1711 NO 1969-5184	19740624 < 19660429 < 19660429 < 19660502 < 19680502 < 19680502 < 19680502 < 19680502 < 19680502 < 19680502 < 19680502 <
	NO 134240 NO 134894	В	19760927	NO 1969-5180	19691231 <

```
В
                                    19760927 NO 1969-5181
19760927 NO 1969-5183
     NO 134895
                                                                             19691231 <--
                   B
A 1972110,
B 19750224
A 19811201
B 19790212
C 19790716
B 19790226
C 19790813
B 19790312
C 19790903
B 19790312
C 19790903
B 19790312
C 19790903
B 19790319
C 19790903
B 19790319
C 19790903
B 19790813
C 19791203
B 19790813
C 19800114
B 19790813
C 19800114
                            В
     NO 134896
                                                                             19691231 <--
     US 3702253
                                                 US 1970-70560
                                                                            19700908 <--
     JP 50004736
                                    19750224
                                                  JP 1971-19574
                                                                             19710330 <--
     US 4303689
                                                 US 1972-243850
                                                                             19720413 <--
     DK 139374
                                                  DK 1973-5432
                                                                             19731005 <--
     DK 139374
     DK 139454
                                                  DK 1973-5428
                                                                             19731005 <--
     DK 139454
     DK 139553
                                                  DK 1973-5429
                                                                             19731005 <--
     DK 139553
     DK 139551
                                                  DK 1973-5430
                                                                             19731005 <--
     DK 139551
     DK 139552
                                                  DK 1973-5431
                                                                             19731005 <--
     DK 139552
     DK 139605
                                                  DK 1973-5426
                                                                             19731005 <--
     DK 139605
     DK 140243
                                                  DK 1973-5427
                                                                             19731005 <--
     DK 140243
     DK 140361
                                                  DK 1973-5433
                                                                             19731005 <--
     DK 140361
     DK 140362
                                                 DK 1973-5434
                                                                             19731005 <--
                            C
A
                                 19800..
19750819
Plteri
     DK 140362
     US 3900582
                                                 US 1974-482818
                                                                             19740624 <--
     Phenolic compds. enhancing or altering the flavor of beverages made from
AΒ
     soluble coffee are described. Flavor characteristics in sirup of coffee
     bases are tabulated for: 2-ethylphenol [90-00-6], 3-ethylphenol
     [620-17-7], 4-ethylphenol [123-07-9], 4-isopropylphenol [99-89-8],
     2,3-xylenol [526-75-0], 2,4-xylenol [105-67-9], 2,5-xylenol [95-87-4],
     2,6-xylenol [576-26-1], 3,4-xylenol [95-65-8], 3,5-xylenol [108-68-9],
     2-hydroxyacetophenone [582-24-1], 2-hydroxypropiophenone [610-99-1],
     4-hydroxypropiophenone [70-70-2], 5-methyl-2-hydroxyacetophenone
     [1450-72-2], 2,3,5-trimethylphenol [697-82-5], 2,4,6-trimethylphenol
     [527-60-6], 2,4,5-trimethylphenol [496-78-6], 3,4,5-trimethylphenol
     [527-54-8], 4-ethyl-2-methoxyphenol [2785-89-9], 4-propyl-2-methoxyphenol
     [2785-87-7], and 4-\text{vinyl-1}, 2-\text{dimethoxybenzene}. . .
ST
     coffee flavoring phenolic
ΙT
     Coffee
         (flavoring materials for)
     Flavoring materials
         (for coffee)
ΙT
     70-70-2 90-00-6 95-65-8 95-87-4 99-89-8 105-67-9 108-68-9
     123-07-9 496-78-6 526-75-0 527-54-8 527-60-6 576-26-1
     582-24-1 610-99-1 620-17-7 697-82-5 1450-72-2 2785-87-7
     2785-89-9 6380-23-0
     RL: BIOL (Biological study)
         (flavoring, for coffee)
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
                                   (2 CITINGS)
ΤI
     Flavoring agent
PΙ
     US 3947603 19760330
     PATENT NO.
                    KIND
                                    DATE
                                                  APPLICATION NO.
                            ____
                                     _____
                                                  _____
     US 3947603 A 19760330 US 1974-482686
BR 6679143 D0 19730911 BR 1966-179143
CH 566111 A5 19750915 CH 1970-13417
GB 1156487 A 19690625 GB 1966-1156487
NO 134890 B 19760927 NO 1968-108
NO 134891 B 19760927 NO 1968-1709
NO 134892 B 19760927 NO 1968-1710
NO 134893 B 19760927 NO 1968-1711
                                                                             19740624 <--
РΤ
                                                                             19660429 <--
                                                                             19660429 <--
                                                                             19660502 <--
                                                                             19680110 <--
                                                                            19680502 <--
                                                                            19680502 <--
                                                                            19680502 <--
```

```
NO 1969-5184
NO 134240
                    В
                          19760531
                                                             19691231 <--
                          19760927
                                      NO 1969-5180
NO 134894
                    В
                                                             19691231 <--
NO 134895
                    В
                          19760927
                                      NO 1969-5181
                                                             19691231 <--
                   В
NO 134896
                          19760927
                                      NO 1969-5183
                                                             19691231 <--
US 3702253
                   Α
                          19721107
                                      US 1970-70560
                                                             19700908 <--
                   В
JP 50004736
                          19750224
                                      JP 1971-19574
                                                             19710330 <--
US 4303689
                   Α
                          19811201
                                      US 1972-243850
                                                             19720413 <--
DK 139374
                                      DK 1973-5432
                   В
                          19790212
                                                             19731005 <--
                   С
DK 139374
                          19790716
DK 139454
                   В
                          19790226
                                      DK 1973-5428
                                                             19731005 <--
DK 139454
                   С
                          19790813
DK 139553
                   В
                          19790312
                                      DK 1973-5429
                                                             19731005 <--
DK 139553
                   С
                          19790903
DK 139551
                   В
                          19790312
                                      DK 1973-5430
                                                             19731005 <--
DK 139551
                   С
                          19790903
DK 139552
                   В
                          19790312
                                      DK 1973-5431
                                                             19731005 <--
DK 139552
                   С
                          19790827
DK 139605
                   В
                          19790319
                                      DK 1973-5426
                                                             19731005 <--
DK 139605
                   С
                          19790903
                   В
DK 140243
                          19790716
                                      DK 1973-5427
                                                             19731005 <--
                   С
DK 140243
                          19791203
                   В
DK 140361
                          19790813
                                      DK 1973-5433
                                                             19731005 <--
                    С
DK 140361
                          19800114
DK 140362
                    В
                          19790813
                                      DK 1973-5434
                                                             19731005 <--
DK 140362
                    С
                          19800114
                          19750819
US 3900582
                                     US 1974-482818
                                                             19740624 <--
                    Α
Phenolic compds. enhancing or altering the flavor of beverages made from
soluble coffee are described. Flavor characteristics in sirup of coffee
bases are tabulated for: 2-ethylphenol [90-00-6], 3-ethylphenol
[620-17-7], 4-ethylphenol [123-07-9], 4-isopropylphenol [99-89-8],
2,3-xylenol [526-75-0], 2,4-xylenol [105-67-9], 2,5-xylenol [95-87-4],
2,6-xylenol [576-26-1], 3,4-xylenol [95-65-8], 3,5-xylenol [108-68-9],
2-hydroxyacetophenone [582-24-1], 2-hydroxypropiophenone [610-99-1],
4-hydroxypropiophenone [70-70-2], 5-methyl-2-hydroxyacetophenone
[1450-72-2], 2,3,5-trimethylphenol [697-82-5], 2,4,6-trimethylphenol
[527-60-6], 2,4,5-trimethylphenol [496-78-6], 3,4,5-trimethylphenol
```

[527-54-8], 4-ethyl-2-methoxyphenol [2785-89-9], 4-propyl-2-methoxyphenol

ST coffee flavoring phenolic

IT Coffee

AB

(flavoring materials for)

IT Flavoring materials

(for coffee)

ΙT 70-70-2 90-00-6 95-65-8 95-87-4 99-89-8 105-67-9 108-68-9 123-07-9 496-78-6 526-75-0 527-54-8 527-60-6 576-26-1 582-24-1 610-99-1 620-17-7 697-82-5 1450-72-2 2785-87-7 2785-89-9 6380-23-0

[2785-87-7], and 4-vinyl-1, 2-dimethoxybenzene [6380-23-0].

RL: BIOL (Biological study)
 (flavoring, for coffee)